



# NON-MARKOVIAN OPEN QUANTUM SYSTEMS

by

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# Abstract

We examine different nonlinear open quantum systems and calculate the non-Markovianity based on the distinguishability between two density matrices. We show that for a single spin (qubit) coupled to a bosonic field the non-Markovianity depends on the spectral density function and can take on any number  $N$  with  $0 \leq N \leq \infty$ , meaning the dynamics can be Markovian or highly non-Markovian. For the main result we consider a system of  $N_{\text{tot}}$  identical spins coupled to an environment in the mean-field way. Each spin is coupled to a local and the common reservoir. There are only indirect interactions between the spins through the common reservoir. In limit  $N_{\text{tot}} \rightarrow \infty$  the subsystem consisting of a fixed set of  $n$  particles reduces to a factorized state in which each factor is a single spin evolving according to a nonlinear Hartree-Lindblad equation which is exactly solvable. For non-stationary initial spin states the non-Markovianity diverges. In this instance we can never approximate the dynamics of the quantum system by a Markovian master equation and this implies that in the mean field models, memory effects are significant.

To my Father

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# Statement of contribution

This thesis is a collaboration of work by Maike Zinterl and Dr. Marco Merkli. The research question investigated throughout the thesis was proposed by Dr. Marco Merkli. The thesis itself was written by Maike Zinterl with the input and guidance of Dr. Marco Merkli. Supervision and editing of the thesis was done by Dr. Marco Merkli.

# Lay summary

In the first part of the thesis we consider a single spin coupled to different environments (chapter 2). The dynamics is described by the Schrödinger equation of the spin plus the environment as dictated by a Hamiltonian containing an interaction term which is energy conserving (conserving the spin energy). We do not make assumptions or simplifications to the Schrödinger equation. The energy conserving interaction allows us to find the exact reduced evolution of the spin by tracing out all environment degrees of freedom.

We consider three environment models: a single quantum harmonic oscillator, finitely many independent oscillators and a free bosonic field (a continuum of oscillators, e.g. a quantized electromagnetic field occupying physical space  $\mathbb{R}^3$ ). After solving the dynamics explicitly we analyze the non-Markovianity of the dynamics (chapter 3). For this we use the definition of the increase of distinguishability between two initial states during the evolution. We characterize the non-Markovianity by the real number  $0 \leq N \leq \infty$ , where  $N = 0$  means that the system is totally Markovian and no memory effects are present.

The physical characteristics of a free field and those of finitely many oscillators are vastly different. For the free field the effective quantum dynamics for the qubit is irreversible while in the latter case it is periodic in time.

For the periodic effective spin quantum dynamics, when the qubit is coupled to finitely many oscillators, there is an everlasting exchange of information between the qubit and its environment in both directions. This results in highly non-Markovian dynamics. We show that in this case we have  $N = \infty$  and memory effects are present.

We would expect the free field to absorb energy and information of the qubit and lose information due to the spatial extension to infinity of the field (modeled by the continuum of quantum oscillators), thereby suppressing memory effects. Intuitively this would result in an approximately Markovian system, i.e.  $N \approx 0$ . Against our intuition though we show that this is not always the case but depends on finer properties of the qubit-environment interaction. This interaction is determined by the so-called spectral

density function  $J(\omega)$ , a function of the reservoir frequency  $\omega$ . It determines which reservoir modes frequencies are available for the interaction with the qubit. Large values of  $J(\omega)$  means the oscillators with frequency  $\omega$  interact strongly with the qubit.

We show that for different spectral density functions the quantity  $N$  of non-Markovianity can take on values between  $0 \leq N \leq \infty$ . Choosing a strong coupling to low energy frequencies (‘infra-red’) with either hard,  $J(\omega) \propto \omega \chi(\omega \leq \omega_0)$ , or exponential cutoff,  $J(\omega) \propto \omega e^{-\omega/\omega_0}$  for some cutoff  $\omega_0 > 0$ , leads to a Markovian dynamics ( $N = 0$ ). On the other hand if the spectral density suppresses the low energy frequencies in the interaction we get a non-Markovian dynamics. For exponential cutoff  $J(\omega) \propto \omega^3 e^{-\omega/\omega_0}$  we get a finite measure ( $N \approx 0.06$ ), while for a hard frequency cutoff,  $J(\omega) \propto \omega^3 \chi(\omega \leq \omega_0)$ , we get a highly non-Markovian dynamics ( $N = \infty$ ). So the interaction with high frequency modes tends to decrease non-Markovianity.

In the second part of the thesis (chapter 4) we consider a system of  $N_{\text{tot}}$  identical spins coupled to an environment in the mean-field way. Each spin is coupled to a local and the common reservoir, all represented by free bosonic quantum fields. In the limit  $N_{\text{tot}} \rightarrow \infty$  the subsystem of  $n$  fixed particles becomes a factorized state (“quantum De Finetti” phenomenon) and each single spin evolves according to a nonlinear Hartree-Lindblad equation which is exactly solvable. We show that the single spin evolution following the Hartree-Lindblad dynamics is highly non-Markovian (meaning that  $N = \infty$ ). In the Hartree-Lindblad equation (4.11) we see that a single qubit is impacted in two ways by its environment. One effect is caused by the local quantum field and the other by all other qubits ( $N_{\text{tot}} - n$ , with  $N_{\text{tot}} \rightarrow \infty$ ). Contrary to the first part of the thesis where the local quantum field contributed to a highly non-Markovian dynamics, here the other qubits produce the memory effects and generate the highly non-Markovian dynamics.

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# Chapter 1

## Introduction

Physics aims to describe systems as close as possible to Nature. Taking this into account we note that it is generally impossible to isolate a specific quantum system from its environment. Therefore we must consider the effects the environment has on the quantum system to realistically model the time evolution of the quantum system. This leads us to the concept of open quantum system. A quantum system is characterized by its unique quantum features such as superposition and coherence. In an open quantum system though we have interactions with the environment which leads to the loss of these unique features, resulting in decoherence and disappearance of quantum superposition. For open systems we generally need a different type of formalism than a Schrödinger equation to describe open quantum systems [6]. Open quantum systems are widely used in applications of quantum physics (i.e. quantum optics [10], quantum biology [25] or quantum chemistry [29]) and are mostly represented by a dynamical semigroup and a corresponding master equation in Lindblad form [19]. These quantum systems are in general very complex and very difficult to solve analytically or numerically. To circumvent the complexity of the equation of motion one usually makes simplifications and approximations for the master equations: The Born-Markov approximation. The Born approximation assumes that the density operator of the full system  $S + E$  factorizes at all times  $t$ ,  $\rho(t) = \rho_S(t) \otimes \rho_E$ . This approximation is reasonable if the action of  $S$  on  $E$  is negligible, so that only the state of  $S$  changes, but not that of  $R$ . The Born approximation is valid if the size of  $E$  is much larger than that of  $S$  and the coupling constant is not too large. In situations where  $E$  is not large enough and  $S$  and  $E$  interact strongly, one cannot expect this approximation to hold. We also assume that the environment  $E$  is large in comparison to the system  $S$  and is

unaffected by the system  $S$ . Additionally we suppose that the interaction between the systems  $S$  and  $E$  described by  $H_I$  is weak. The Markov approximation is based on the fact that the future state  $\rho_S(t)$  for  $t > 0$  is only dependent on the present state  $\rho_S(0)$  and not on its history. This means we have no memory effects.

These systems are widely accepted in many cases and understood quite well but there do exist systems where the Born-Markov approximations are not justified. A Markovian approximation can hide crucially quantum effects such as systems interacting strongly with its environment or when memory effects are present.

Much effort and many techniques have been invested in this theory, but full understanding is yet to be reached. This is where the question arises how one can define non-Markovianity, measure it and how does it manifest itself in the quantum case? Different definitions and measures for non-Markovianity have been introduced [5, 27, 20, 16] and compared [1]. Definitions of quantum Markovian dynamics include the following: distinguishability measure (by Breuer, Laine and Piilo [5]), divisibility measure (by Rivas, Huelga and Plenio [27]), coherent information measure (by Luo, Fu and Song [21]) and channel capacity measures (by Bylicka, Chruściński and Maniscalco [8]). The different criteria for Markovian dynamics are not equivalent [17]. Consensus about a universal definition for quantum (non-) Markovian dynamics is not yet achieved.

In this thesis I will focus on the quantitative measure  $N(\Phi)$  for non-Markovianity introduced by Breuer et. al. [5] for open quantum systems. The measure relies on the trace distance  $D(t, \rho, \nu)$  between two quantum states  $\rho$  and  $\nu$  and its change over time. A Markovian process is characterized by a monotonic decrease of the trace distance for all initial quantum states over time while a non-Markovian process has at least one pair of quantum states for which the trace distance increases for some time  $t > 0$ .

- The results in section 3.3 with spectral density function  $J(\omega) = \frac{\omega^s}{\omega_0^{s-1}} e^{-\omega/\omega_0}$  and  $s > 0$  has been considered in [14, 13, 1]. However we consider a new spectral density function  $J(\omega) = \pi \omega^s \chi(\omega \leq \omega_0)$  in 3.3, which has not been considered before, to our knowledge.
- The results in section 4.2 have been obtained in [24]. However the calculation of the non-Markovianity in section 4.3 is new to our knowledge.

## 1.1 Open Quantum systems

Following [2] and [4] we introduce some notions and general concepts of open quantum systems.

In the following we consider an open quantum system  $S$  with its associated Hilbert space  $\mathcal{H}_S$ . A state  $\rho_S(t)$  of the quantum system  $S$  changes due to internal dynamics and interactions with the environments  $E$  with its associated Hilbert Space  $\mathcal{H}_E$ . The Hilbert space of the total system  $S + E$  is given by the tensor product state

$$\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E. \quad (1.1)$$

Physical states of the total system  $\mathcal{H}$  are described by density matrices  $\rho(t)$ <sup>1</sup>. To arrive at the states of the subsystems  $S$  and  $E$  we take the partial trace over  $\mathcal{H}_E$  and  $\mathcal{H}_S$  respectively, i.e.  $\rho_S(t) = \text{Tr}_E(\rho(t))$  and  $\rho_E(t) = \text{Tr}_S(\rho(t))$ . We call  $\rho_S(t)$  the reduced density matrix of the quantum system  $S$ .

**Definition 1.1.1.** A density matrix  $\rho(t)$  is a positive, trace class operator on  $\mathcal{H}$  with unit trace, i.e.

1.  $\text{Tr}(\rho(t)) = 1 \ \forall t$
2.  $\langle \psi | \rho(t) | \psi \rangle \geq 0, \ \forall \psi \in \mathcal{H}$ . (short  $\rho(t) \geq 0$ )
3.  $\rho(t) = \rho(t)^*$ .

The convex set of all physical states belonging to the Hilbert space  $\mathcal{H}$  is denoted by  $\mathcal{S}(\mathcal{H})$  and called state space. By  $\partial\mathcal{S}(\mathcal{H})$  we denote the boundary of  $\mathcal{S}(\mathcal{H})$ .

**Remark 1.1.2.** From the positive semidefinite characteristic of a density matrix

$$\rho = \begin{pmatrix} p & c \\ c^* & 1-p \end{pmatrix} \quad (1.2)$$

it follows that

$$\sqrt{p(1-p)} \geq |c| \quad (1.3)$$

and  $p \in [0, 1]$ .

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<sup>1</sup>For more detail on density matrices and its concept as physical states see e.g. [6].

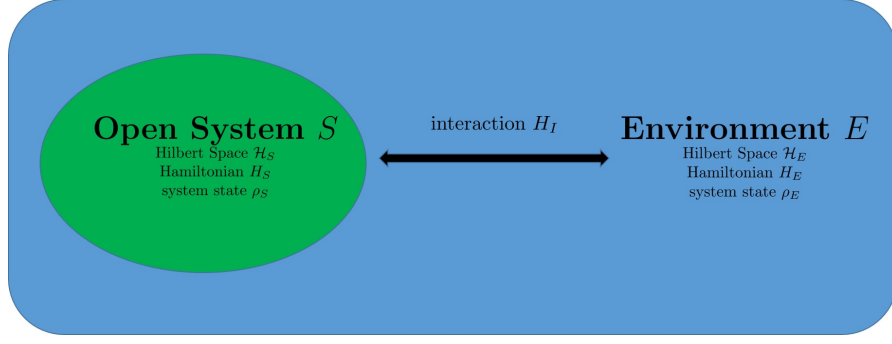


Figure 1.1: Open quantum system

Sketch of an open quantum system  $S$  which is coupled to an environment  $E$  via the interaction Hamiltonian  $H_I$  (see [4]).

We assume that the total system  $S+E$  is closed and follows unitary dynamics described by some unitary time evolution operator <sup>2</sup>

$$U(t) = e^{-itH}. \quad (1.4)$$

The Hamiltonian in its most general form is then given by

$$H = H_S \otimes \mathbb{1}_E + \mathbb{1}_S \otimes H_E + H_I, \quad (1.5)$$

where  $H_S$  and  $H_E$  are the free Hamiltonians of the systems  $S$  and  $E$ , and  $H_I$  is the interaction Hamiltonian (see figure 1.1).

The dynamics of the total system is thus obtained from the Liouville-von Neumann equation (see for example [6] p. 106)

$$\frac{d}{dt}\rho(t) = -i[H, \rho(t)], \quad (1.6)$$

with the formal solution

$$\rho(t) = U(t)\rho(0)U^*(t) \quad (1.7)$$

and with  $U(t)$  given in (1.4).

---

<sup>2</sup>We set  $\hbar = 1$  throughout the thesis.

### 1.1.1 Quantum dynamical maps

There exist a variety of methods to treat open quantum systems. In this thesis we will focus on the description through a dynamical map. From here on we assume the following

1. the dynamics of the total system  $\mathcal{H}$  is given by a unitary time evolution (1.7)
2. we are able to prepare, at a time  $t_0 = 0$ , the initial state of the total system as an uncorrelated product state

$$\rho(0) = \rho_S(0) \otimes \rho_E(0), \quad (1.8)$$

where  $\rho_S(0)$  is a varying initial state of  $S$  and  $\rho_E(0)$  is the fixed reference state of the environment  $E$ .

On the basis of these assumptions we can write the open system state  $\rho_S(t)$  at time  $t \geq 0$  as

$$\rho_S(t) = \text{Tr}_E (U(t) \rho_S(0) \otimes \rho_E(0) U^*(t)), \quad (1.9)$$

where we have taken the partial trace  $\text{Tr}_E$  over the environment. For each  $t \geq 0$ , equation (1.9) defines a linear map

$$\Phi(t, 0) : \mathcal{S}(\mathcal{H}_S) \rightarrow \mathcal{S}(\mathcal{H}_S), \quad (1.10)$$

which maps *any* initial open system state  $\rho_S(0)$  to the corresponding open system state at time  $t$

$$\rho_S(0) \mapsto \rho_S(t) = \Phi(t, 0) \rho_S(0). \quad (1.11)$$

$\Phi(t, 0)$  is called *quantum dynamical map* corresponding to time  $t$  and maps physical states to physical states.

**Definition 1.1.3.** A positive, trace and hermiticity (see references [2] and [4]) preserving map (PTP)  $\Phi$  on  $\mathcal{S}(\mathcal{H}_S)$  is a linear map with the properties:

1.  $\rho \geq 0 \Rightarrow \Phi\rho \geq 0$
2.  $\text{Tr}_S(\Phi\rho) = \text{Tr}_S(\rho)$
3.  $(\Phi\rho)^* = \Phi\rho^*$

**Corollary 1.1.4.** For each  $t$  fixed the quantum dynamical map

$$\begin{aligned} \Phi(t, 0) : \mathcal{S}(\mathcal{H}_S) &\rightarrow \mathcal{S}(\mathcal{H}_S) \\ \rho_S(0) &\mapsto \text{Tr}_E (U(t) \rho_S(0) \otimes \rho_E(0) U^*(t)) = \rho_S(t) \end{aligned} \quad (1.12)$$

with unitary operator  $U(t)$ , is a PTP map.

*Proof.* Let  $\rho_S(0)$  be an arbitrary density matrix, i.e. it fulfills definition 1.1.1.

1.

$$\begin{aligned}\Phi(t, 0)\rho_S(0) &= \text{Tr}_E (U(t)\rho_S(0) \otimes \rho_E(0)U^*(t)) \\ &= \rho_S(t) \geq 0, \quad \text{as } \rho_S(t) \in \mathcal{S}(\mathcal{H}_S)\end{aligned}\tag{1.13}$$

2.

$$\begin{aligned}\text{Tr}_S(\Phi(t, 0)\rho_S(0)) &= \text{Tr}_S \left( \text{Tr}_E (U(t)\rho_S(0) \otimes \rho_E(0)U^*(t)) \right) \\ &= \text{Tr}_S(\rho_S(0))\end{aligned}\tag{1.14}$$

3.

$$\begin{aligned}(\Phi(t, 0)\rho_S(0))^* &= \left( \text{Tr}_E (U(t)\rho_S(0) \otimes \rho_E(0)U^*(t)) \right)^* \\ &= (\rho_S(t))^* = \text{Tr}_E (U(t)(\rho_S(0) \otimes \rho_E(0))^* U^*(t)) \\ &= \Phi(t, 0)(\rho_S(0))^*\end{aligned}\tag{1.15}$$

■

**Remark 1.1.5.** The dynamical map  $\Phi(t, 0)$  is not only positive but actually completely positive<sup>3</sup>. One calls these maps trace preserving quantum operations or quantum channels in quantum information theory.

If we now let  $t$  vary over a time interval  $[0, T]$ , where  $T$  may be finite or infinite, we obtain a one-parameter family of dynamical maps with

$$\{\Phi(t, 0) | 0 \leq t \leq T, \Phi(0, 0) = \Phi_0 = \mathbb{1}\}.\tag{1.16}$$

All information on the future time evolution of all possible initial states is contained in this one-parameter family of dynamical maps. Hence a quantum process of an open system is given by such a one-parameter family of completely positive and trace-preserving (CPT) quantum dynamical maps.

**Example 1.1.6.** Examples for dynamical maps are given by (see [2])

- $\Phi(t, 0)\rho = e^{-itH}\rho e^{itH}$ , the Hamiltonian evolution of a closed system.

---

<sup>3</sup>A linear map  $\Phi$  is completely positive if and only if there exists a Kraus representation [18]. This means that there are operators  $\Omega_i$  on the underlying Hilbert Space  $\mathcal{H}_S$  such that  $\Phi A = \sum_i \Omega_i A \Omega_i^*$ , and that the condition of trace preservation takes the form  $\sum_i \Omega_i \Omega_i^* = \mathbb{1}$ .



- $\Phi(t, 0) = e^{\mathcal{L}t}$ , where  $\mathcal{L}$  is a superoperator<sup>4</sup> with  $Re(\mathcal{L}) \leq 0$ . This is the dissipative evolution of an open system.

### 1.1.2 Trace distance

The measure of non-Markovianity by Breuer is based on the idea of the ability to distinguish between two quantum states  $\rho$  and  $\nu$  (see [5]). In a Markovian process the distinguishability between two quantum states never decreases. In contrast, a non-Markovian process has times such that the distinguishability between two quantum states increases. The trace distance defined in (1.17) gives a measure for distinguishability. We can characterize the decrease or growth of distinguishability as a flow of information between the environment  $S$  and the environment  $E$ . For a Markovian process we for ever lose information from the system to the environment but in a non-Markovian process we have a backflow of information from the environment to the system (see figure 1.2).

**Definition 1.1.7.** The trace distance  $D(\rho, \nu)$  for two quantum states  $\rho$  and  $\nu$  is defined as

$$D(\rho(0), \nu(0)) = \frac{1}{2} \text{Tr} |\rho - \nu|, \quad (1.17)$$

where  $|A| = \sqrt{A^*A}$ . Considering the initial state  $\rho(0)$  which evolves in time to  $\rho(t)$  we define

$$D(t, \rho, \nu) \equiv D(\rho(t), \nu(t)). \quad (1.18)$$

**Remark 1.1.8.** The trace distance gives rise to a natural metric on  $S$  with  $0 \leq D \leq 1$  ([26], p.403ff).

An important feature of the trace distance is that a CPT map  $\Phi$  is a contraction for this metric

$$D(\Phi\rho, \Phi\nu) \leq D(\rho, \nu) \quad \forall \rho, \nu \in S. \quad (1.19)$$

This means that a trace preserving quantum operation reduces or holds the current distinguishability between the two quantum states  $\rho$  and  $\nu$ .

**Definition 1.1.9.** A quantum process is given by a family of quantum dynamical maps (1.16). We consider a quantum process *Markovian* if the trace distance  $D(\rho(t), \nu(t))$  for

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<sup>4</sup>A superoperator is an operator acting on operators, i.e. the dynamical map  $\Phi(t, 0)$  is an operator acting on physical states  $\rho(t)$  which are operators themselves.

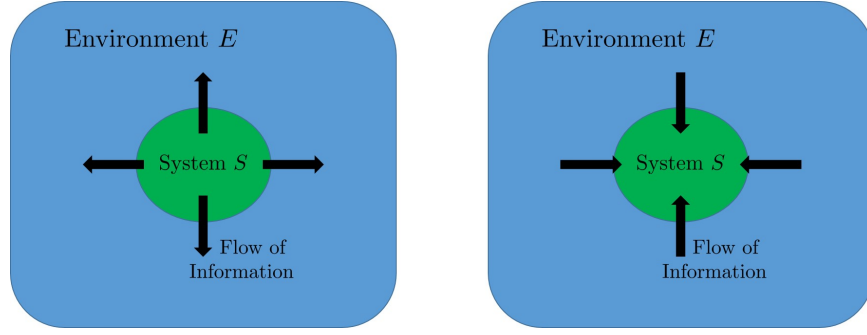


Figure 1.2: Comparison Markovian and non-Markovian process

Left: Markovian process with a flow of information from the system to the environment. Right: Backflow of information for some time interval  $t > 0$  from the environment to the system in a non-Markovian process.

all initial quantum states  $\rho(0)$  and  $\nu(0)$  decreases monotonically for all times  $t > 0$ . We thus have a continuous loss of information from the system  $S$  to the environment  $E$ . In contrast to this we differentiate a quantum *non-Markovian* process through the fact that there exist a pair of initial states  $\rho(0)$  and  $\nu(0)$  such that the trace distance  $D(\rho(t), \nu(t))$  increases for some time  $t > 0$ . We interpret this as backflow of information from the environment to the system.

**Remark 1.1.10.** Interpreting the trace distance as flow of information leads us to the concept of memory effects: In a non-Markovian process information from the system  $S$  is temporarily stored in the environment  $E$  and effects the system  $S$  at some later time.

### 1.1.3 Master equation

Historically only master equations in Lindblad form (1.21) were associated to a Markovian time evolution. All other master equations were considered non-Markovian. If

$$\rho(t) = \Phi(t)\rho_S(0) = e^{\mathcal{L}t}\rho_S(0). \quad (1.20)$$

holds for a  $\Phi$  which is a CPT semigroup<sup>5</sup>, then it is known (Gorini-Kossakowski-Sudarshan-Lindblad theorem) that the generator has to have the form

$$\mathcal{L}\rho = -i[H_S, \rho] + \sum_i \gamma_i [A_i \rho A_i^* - \frac{1}{2} \{A_i^* A_i, \rho\}], \quad (1.21)$$

<sup>5</sup>The semigroup property here is given by:  $\Phi(t + \tau) = \Phi(t)\Phi(\tau)$

with self-adjoint Hamiltonian  $H_S(t)$ , the Lindblad operators  $A_i$  describing the various decay modes of the system and  $\gamma_i \geq 0$  corresponding decay rates. Since  $\mathcal{L}$  is independent of  $t$  we clearly have the semigroup property for this dynamical map

$$\Phi(t)\Phi(\tau) = e^{\mathcal{L}t}e^{\mathcal{L}\tau} = e^{\mathcal{L}(t+\tau)} = \Phi(t+\tau). \quad (1.22)$$

Now using the semigroup property and the fact that a dynamical CPT map is a contraction on the trace distance (see (1.19)) we can conclude that

$$D(\rho(t+s), \nu(t+s)) = D(\Phi(t)\rho(s), \Phi(t)\nu(s)) \leq D(\rho(s), \nu(s)) \quad \forall t \geq s \quad (1.23)$$

for any two initial conditions  $\rho(0)$  and  $\nu(0)$  with  $\rho(s) = \Phi(s)\rho(0)$  and  $\nu(s) = \Phi(s)\nu(0)$ . One can see here that the semigroup property leads us to the conclusion that the trace distance is a monotonically decreasing function of time for this dynamical semigroup. We have defined earlier that a monotonically decrease of the trace distance corresponds to a Markovian dynamics. So the historic definition of Markovian dynamics and our definition are consistent.

Actually the inequality (1.23) not only holds for the quantum dynamics described by master equations of Lindblad form (1.21) but also for master equations in the ‘dynamical’ Schrödinger form

$$\partial_t \rho(t) = K(t)\rho(t), \quad (1.24)$$

where  $K(t)$  is a general time-dependent superoperator. This is a linear first-order differential equation for the open system state  $\rho(t)$ . Given an initial condition  $\rho(0)$ , (1.24) has a unique solution. The generator  $K(t)$  preserves hermiticity and trace, i.e.

$$(K(t)\rho)^* = K(t)\rho^*, \quad (1.25)$$

$$\text{Tr}_S(K(t)\rho) = \text{Tr}_S(\rho). \quad (1.26)$$

From these requirements it follows that the generator must be of the following most general form [11, 3]

$$K(t)\rho = -i[H_S(t), \rho] + \sum_i \gamma_i(t) [A_i(t)\rho A_i^*(t) - \frac{1}{2} \{A_i^*(t)A_i(t), \rho\}]. \quad (1.27)$$

Here the self-adjoint Hamiltonian  $H_S(t)$ , the Lindblad operators  $A_i(t)$  as well as the decay

rates  $\gamma_i(t)$  may depend on time. For this master equation we can write the solution as

$$\rho(t) = \Phi(t, s)\rho(s), \quad t \geq s, \quad (1.28)$$

where now  $\Phi(t, s)$  is a two-parameter group satisfying  $\Phi(t, t) = \mathbb{1}$  and has the divisibility property

$$\Phi(t', s) = \Phi(t', s')\Phi(s', s), \quad t' \geq s' \geq s. \quad (1.29)$$

This dynamical map satisfying the divisibility property (1.29) also leads us to a Markovian process, as it also fulfills inequality (1.23) and thus has a monotonic decrease of the trace distance for all times and all initial quantum states.

## 1.2 Non-Markovianity

We have seen in the previous section that a dynamical Schrödinger equation (1.24) leads to a dynamical semigroup of CPT maps and this in turn leads to a monotonic decrease of the trace distance for any two initial quantum states. This corresponds to an irreversible flow of information from the open system  $S$  to its environment  $E$  in a Markovian process. We want to not only have a physical interpretation of a non-Markovian process but also a quantitative measure for non-Markovianity. For this we define the rate of change of the trace distance

**Definition 1.2.1.** The rate of change of the trace distance  $D(\rho(t), \nu(t))$  is defined by

$$\sigma(t, \rho(0), \nu(0)) := \partial_t D(\rho(t), \nu(t)) \quad \forall t \geq 0. \quad (1.30)$$

Note here that we must specify the initial states  $\rho(0)$  and  $\nu(0)$  to be able to calculate  $\sigma$ .

For a dynamical semigroup  $\Phi(t, s)$  and  $s = 0$  in inequality (1.23) we conclude that

$$\sigma(t, \rho(0), \nu(0)) \leq 0, \quad \forall t \geq 0. \quad (1.31)$$

We now define the violation of inequality (1.31) as the quantitative measure for non-markovianity.

**Definition 1.2.2.** We define the measure for non-markovianity by

$$N(\Phi) := \max_{\rho(0), \nu(0)} \int_{\{t \geq 0: \sigma(t, \rho(0), \nu(0)) > 0\}} \sigma(t, \rho(0), \nu(0)) dt. \quad (1.32)$$

This implies that all divisible quantum maps  $\Phi$  satisfying (1.29) lead to a Markovian process as they always satisfy inequality (1.31). It also entails that for a non-Markovian process we must have a non-divisible quantum map. Note though that there exist non-divisible maps that do not lead to a non-Markovian process. It also follows that  $N(\Phi) = 0$  iff the trace distance  $D(\rho(t), \nu(t))$  is a monotonically decreasing function in time  $t$  for any two initial pairs  $\rho(0), \nu(0)$ . In contrast  $N(\Phi) > 0$  means that there exist an initial pair of states for which the trace distance increases over a certain time interval. A positive measure  $N(\Phi)$  means there is a flow of information from the environment back to the open system at some time. As we take the maximum over all initial state pairs,  $N(\Phi)$  represents the maximal backflow of information.

One can explicitly calculate the trace distance  $D(t, \rho, \nu)$  for a given system  $S$  and a local time master equation.

**Lemma 1.2.3.** *Given a two level quantum dynamical process,  $\dim(\mathcal{H}_S) = 2$ , and two quantum states  $\rho$  and  $\nu$  the trace distance  $D(\rho, \nu)$  is given by*

$$D(\rho, \nu) = \sqrt{\alpha(t)^2 + |v(t)|^2}, \quad (1.33)$$

where

$$\alpha = \rho_{11} - \nu_{11} \quad (1.34)$$

$$v = \rho_{12} - \nu_{12}. \quad (1.35)$$

Here the general density matrix  $\rho$  is given by

$$\rho = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} \in \mathcal{H}_S. \quad (1.36)$$

*Proof.* First, note that since  $\rho$  is a density matrix we have  $\rho_{21} = \rho_{12}^*$  and  $\rho_{22} = 1 - \rho_{11}$ . Thus

$$\rho = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{12}^* & 1 - \rho_{11} \end{pmatrix}, \quad (1.37)$$

and equivalently for the state  $\nu$ .

Set

$$\rho - \nu = \begin{pmatrix} \alpha & v \\ v^* & -\alpha \end{pmatrix}, \quad (1.38)$$

where

$$\alpha = \rho_{11} - \nu_{11} \quad (1.39)$$

$$v = \rho_{12} - \nu_{12}. \quad (1.40)$$

Using the definition for the trace distance (1.17)  $D(\rho, \nu) = \frac{1}{2} \text{Tr} |\rho - \nu|$ , we calculate

$$|\rho - \nu| = \sqrt{(\rho - \nu)^2}. \quad (1.41)$$

Then

$$(\rho - \nu)^2 = (\alpha^2 + |v|^2) \mathbb{1} \quad (1.42)$$

is a diagonal matrix.

$$\Rightarrow |\rho - \nu| = \sqrt{(\alpha^2 + |v|^2)} \mathbb{1} \quad (1.43)$$

Then (1.33) follows with equations (1.39) and (1.40) and  $\text{Tr} |\rho - \nu| = 2 \cdot \sqrt{\alpha^2 + |v|^2}$ . ■

For a qubit system (i.e.  $\dim \mathcal{H}_S = 2$ ) we can also give an explicit formula for the time derivative  $\sigma$ .

**Lemma 1.2.4.** *With the same assumptions as in Lemma 1.2.3 we have*

$$\sigma(t, \rho, \nu) = \frac{\alpha(t)\alpha'(t) + \text{Re}(v'(t)v^*(t))}{\sqrt{\alpha^2(t) + |v(t)|^2}}. \quad (1.44)$$

*Proof.* Take the time derivative of equation (1.33) with, recall  $\alpha(t) = \rho_{11}(t) - \nu_{11}(t)$  and  $v(t) = \rho_{12}(t) - \nu_{12}(t)$ :

$$\begin{aligned} \sigma(t, \rho, \nu) &= \partial_t \sqrt{\alpha(t)^2 + |v(t)|^2} \\ &= \frac{2\alpha(t)\alpha'(t) + v'(t)v^*(t) + v(t)(v'(t))^*}{2\sqrt{\alpha^2(t) + |v(t)|^2}} \\ &= \frac{\alpha(t)\alpha'(t) + \text{Re}(v'(t)v^*(t))}{\sqrt{\alpha^2(t) + |v(t)|^2}}. \end{aligned} \quad (1.45)$$

■

### 1.2.1 Example for non-Markovian dynamics

An example of when  $\sigma(t, \rho, \nu)$  can be positive for a master equation of form (1.24) is calculated in the following. Motivational work can be found in [5].

**Example 1.2.5.** Consider a two level system governed by the dynamical Schrödinger equation (1.24) with

$$K(t)\rho = \gamma(t) [A\rho A^* - \frac{1}{2} \{A^*A, \rho\}] , \quad (1.46)$$

where  $A$  is the annihilation and  $A^*$  the creation operator and  $\gamma(t)$  a real function. We have the following properties for  $A$  and  $A^*$  acting on the excited  $|+\rangle$  and ground  $|-\rangle$  states <sup>6</sup>

$$\begin{aligned} A|+\rangle &= |-\rangle \\ A|-\rangle &= 0 \\ A^*|+\rangle &= 0 \\ A^*|-\rangle &= |+\rangle . \end{aligned} \quad (1.47)$$

The general density matrix  $\rho(t)$  is of the form

$$\rho(t) = \begin{pmatrix} p(t) & c(t) \\ c^*(t) & 1 - p(t) \end{pmatrix} . \quad (1.48)$$

Thus

$$\partial_t \rho(t) = \dot{\rho}(t) = \begin{pmatrix} \dot{p}(t) & \dot{c}(t) \\ \dot{c}^*(t) & -\dot{p}(t) \end{pmatrix} . \quad (1.49)$$

Taking the matrix element  $\langle + | \cdot | + \rangle$  of the master equation

$$\partial_t \rho(t) = \gamma(t) [A\rho A^* - \frac{1}{2} \{A^*A, \rho\}] \quad (1.50)$$

and using the properties (1.47) for the creation and annihilation operators we have for the l.h.s. (left hand side) and r.h.s. (right hand side)

**l.h.s.:**

$$\langle + | \partial_t \rho(t) | + \rangle = \dot{p}(t)$$

---

<sup>6</sup>One can associate the vectors  $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$  and  $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$  with  $|+\rangle$  and  $|-\rangle$ .

**r.h.s.:**

$$\begin{aligned}
\langle + | K(t) \rho(t) | + \rangle &= \gamma(t) \langle + | A \rho A^* | + \rangle - \frac{\gamma(t)}{2} \langle + | A^* A \rho + \rho A^* A | + \rangle \\
&= 0 - \frac{\gamma(t)}{2} (\langle + | A^* A \rho | + \rangle + \langle + | \rho A^* A | + \rangle) \\
&= -\frac{\gamma(t)}{2} (\langle + | \rho | + \rangle + \langle + | \rho | + \rangle) \\
&= -\frac{\gamma(t)}{2} (p(t) + p(t)) \\
&= -\gamma(t) p(t)
\end{aligned}$$

Thus we arrive at the differential equation

$$\dot{p}(t) = -\gamma(t) p(t). \quad (1.51)$$

Now take the  $\langle + | \cdot | - \rangle$  matrix element of (1.50) and we have for the l.h.s. and r.h.s.:

**l.h.s.:**

$$\langle + | \partial_t \rho(t) | - \rangle = \dot{c}(t) \quad (1.52)$$

**r.h.s.:**

$$\begin{aligned}
\langle + | K(t) \rho(t) | - \rangle &= \gamma(t) \langle + | A \rho A^* | - \rangle - \frac{\gamma(t)}{2} \langle + | A^* A \rho + \rho A^* A | - \rangle \\
&= \gamma(t) \langle + | A | \rho | + \rangle - \frac{\gamma(t)}{2} (\langle + | A^* A \rho | - \rangle + \langle + | \rho A^* A | - \rangle) \\
&= -\frac{\gamma(t)}{2} \langle + | A \rho | - \rangle \\
&= -\frac{\gamma(t)}{2} \langle + | \rho | - \rangle \\
&= -\frac{\gamma(t)}{2} c(t)
\end{aligned}$$

The second differential equation is then given by

$$\dot{c}(t) = -\frac{\gamma(t)}{2} c(t). \quad (1.53)$$

Set

$$\Gamma(t) = \int_0^t \gamma(s) ds.$$

Solving (1.51) and (1.53) (excluding  $p(t) = c(t) = 0$  here), yields

$$p(t) = e^{-\Gamma(t)} p(0) \quad (1.54)$$

$$c(t) = e^{-\frac{1}{2}\Gamma(t)} c(0). \quad (1.55)$$



Note that if  $p(t) = 0$  and  $c(t) = 0$  we have the trivial stationary solution

$$\rho(t) = \rho = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad (1.56)$$

and this clearly satisfies equation (1.50).

We set

$$z(t) = e^{-\frac{1}{2}\Gamma(t)}$$

so that

$$\rho(t) = \begin{pmatrix} z^2(t)p(0) & z(t)c(0) \\ z(t)c(0)^* & 1 - z^2(t)p(0) \end{pmatrix}. \quad (1.57)$$

Now consider the two initial conditions

$$\nu(0) = |-\rangle \langle -| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \text{ and } \rho(0) = |+\rangle \langle +| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \quad (1.58)$$

These are two initial quantum states and we can thus calculate the unique solutions for the differential equations (1.51) and (1.53). For the initial density matrix  $\rho(0)$  with  $t = 0$  we have

$$\begin{aligned} z^2(0)p(0) &\stackrel{!}{=} 1 \\ \Rightarrow e^{-\Gamma(0)}p(0) &= 1 \\ \Rightarrow p(0) &= 1 \end{aligned}$$

and

$$\begin{aligned} z(t=0)c(0) &\stackrel{!}{=} 0 \\ \Rightarrow e^{-\Gamma(0)}c(0) &= 0 \\ \Rightarrow c(0) &= 0. \end{aligned}$$

With (1.54) and (1.55)

$$p(t) = e^{-\Gamma(t)} \quad (1.59)$$

$$c(t) = 0 \quad (1.60)$$

follows. So for the evolved density matrix  $\rho(t)$  at time  $t$  with the initial state  $\rho(0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$

we have

$$\rho(t) = \begin{pmatrix} z^2(t) & 0 \\ 0 & 1 - z^2(t) \end{pmatrix}. \quad (1.61)$$

Similarly we have for the evolved density matrix  $\nu(t)$  the following initial conditions at time  $t = 0$

$$\begin{aligned} z^2(0)p(0) &\stackrel{!}{=} 0 \quad \text{and} \\ z(0)c(0) &\stackrel{!}{=} 0 \\ \Rightarrow p(0) &= c(0) = 0 \end{aligned}$$

and thus with (1.54) and (1.55)

$$p(t) = c(t) = 0 \quad (1.62)$$

follows. This results in

$$\nu(t) = \nu(0) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad (1.63)$$

for the evolved density matrix  $\nu(t)$ . Using Lemma (1.2.3) we have

$$\begin{aligned} D(t, \rho, \nu) &= \sqrt{(\rho_{11}(t) - \nu_{11}(t))^2 + |\rho_{12}(t) - \nu_{12}(t)|^2} \\ &= \sqrt{(z^2(t))^2} \\ &= z^2(t) \\ &= e^{-\Gamma(t)} \end{aligned}$$

and

$$\sigma(t, \rho(0), \nu(0)) = -\gamma(t)e^{-\Gamma(t)} \quad (1.64)$$

with

$$\Gamma(t) = \int_0^t \gamma(s)ds. \quad (1.65)$$

Choosing  $\gamma(t)$  such that for some time  $t > 0$  we have  $\gamma(t) < 0$  results in  $\sigma(t) > 0$  for  $t \in (a, b)$ . We have found explicit initial quantum states  $\rho(0), \nu(0)$  such that for some time  $t \in (a, b)$  <sup>7</sup> the trace distance  $D(t, \rho, \nu)$  and the distinguishability between the states  $\rho(t)$  and  $\nu(t)$  increases. The master equation (1.46) thus describes a non-Markovian process.

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<sup>7</sup>The time interval  $(a, b)$  can be just one interval with  $b > a > 0$  or a countable number of intervals  $(a_i, b_i)$ ,  $i \in \mathbb{N}$  with  $b = \infty$  possible.

With (1.32) and a given decay rate  $\gamma(t)$  we can explicitly calculate the measure  $N(\Phi)$

$$\begin{aligned} N(\Phi) &= \max_{\rho(0), \nu(0)} \int_{\gamma(t) < 0} -\gamma(t) e^{-\Gamma(t)} dt \\ &= \max_{\rho(0), \nu(0)} \sum_i e^{-\Gamma(b_i)} - e^{-\Gamma(a_i)}, \end{aligned} \tag{1.66}$$

where  $(a_i, b_i)$  are the time intervals with  $\gamma(t) < 0$ .

# Chapter 2

## Spin Boson model

In this chapter we consider the spin boson model. As our open system  $S$  we take a  $\frac{1}{2}$  spin, also called a qubit system. The qubits Hilbert space is  $H_S = \mathbb{C}^2$ . For the environment we examine three different cases

1. Spin coupled to a single quantum harmonic oscillator mode
2. Spin coupled to a multitude of quantum harmonic oscillators
3. Spin coupled to a free bosonic field.

The goal is to find the explicit reduced density matrix  $\rho_S(t)$ , which we can calculate using (compare to section [1.1.3](#))

$$\rho_S(t) = \text{Tr}_E(e^{-itH}(\rho_S(0) \otimes \rho_E)e^{itH}), \quad (2.1)$$

for the given Hamiltonian  $H$  in each case. We also use the widely known creation  $a^*$  and annihilation  $a$  operators ( for a mathematical description see [\[22\]](#)) satisfying the canonical commutation relations (CCR)  $[a, a^*] = aa^* - a^*a = \mathbb{1}$ , where these operators act on the Hilbert space  $\mathcal{H}_{osc}$  of a single harmonic oscillator. Here,  $\rho_S(0)$  is an arbitrary initial spin density matrix of the system  $S$ ,  $\xi$  a complex number and  $\rho_E$  the equilibrium density matrix for a single harmonic oscillator at inverse temperature  $\beta$ , which satisfies

$$\text{Tr}_E(\rho_E e^{i(\xi a^* + \xi^* a)}) = e^{-\frac{1}{2}|\xi|^2 \coth(\beta\omega/2)}. \quad (2.2)$$

We need in the following several operators which we will define here.

**Definition 2.0.1.** The operator  $P_1 = |\uparrow\rangle\langle\uparrow|$  is the projection onto the spin up state, whereas  $P_2 = |\downarrow\rangle\langle\downarrow|$  is the projection onto the spin down state and

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (2.3)$$

$$P_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad (2.4)$$

$$P_2 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \quad (2.5)$$

It follows with easy calculation that

$$\sigma_z P_1 = P_1 \quad (2.6)$$

$$(P_1 \otimes \mathbb{1})^n = P_1 \otimes \mathbb{1}, \quad \forall n \in \mathbb{N}, \quad (2.7)$$

where  $\mathbb{1}$  is the identity operator on  $\mathcal{H}_{osc}$ . Later we will need the following definition.

**Definition 2.0.2.** We define the complex numbers  $c_{ij}$  as

$$c_{ij} = \text{Tr}_E(e^{-itH_i} \rho_E e^{itH_j}), \quad (2.8)$$

where the operators  $H_i$  and  $H_j$  are operators acting on the Hilbert space  $\mathcal{H}_{osc}$ .

## 2.1 Spin coupled to single harmonic oscillator

A spin is coupled to a single quantum harmonic oscillator mode, with Hamiltonian

$$H = \frac{\epsilon}{2} \sigma_z + \omega a^* a + \frac{\lambda}{2} \sigma_z \otimes (a^* + a) \quad \lambda, \omega, \epsilon \in \mathbb{R}. \quad (2.9)$$

The operator acts on the Hilbert space  $\mathbb{C}^2 \otimes \mathcal{H}_{osc}$ , where  $\mathcal{H}_{osc}$  is the Hilbert space of the quantum harmonic oscillator. Physically, (2.9) describes a two-level system interacting with a harmonic oscillator (a "spring") at oscillating frequency  $\omega > 0$ ,  $\epsilon$  is the energy difference of the 2 levels and  $\lambda$  the coupling strength.

For the reduced density matrix  $\rho_S(t)$  we claim:

$$\begin{aligned}
\rho_S(t) &= \text{Tr}_E(e^{-itH}(\rho(0) \otimes \rho_E)e^{itH}) \\
&= \sum_{i,j \in \{1,2\}} c_{ij} P_i \rho(0) P_j,
\end{aligned} \tag{2.10}$$

where  $c_{ij}$  is defined in equation (2.8), with  $H_1, H_2$  given below in 2.12 and 2.18. For this we first show

$$H(P_1 \otimes \mathbb{1}) = P_1 \otimes H_1 \tag{2.11}$$

with

$$H_1 = \frac{\epsilon}{2} \mathbb{1} + \omega a^* a + \frac{\lambda}{2} (a^* + a) \tag{2.12}$$

being an operator on  $\mathcal{H}_{osc}$ . Using (2.6) we calculate

$$\begin{aligned}
(P_1 \otimes \mathbb{1})H &= (P_1 \otimes \mathbb{1}) \left[ \frac{\epsilon}{2} \sigma_z \otimes \mathbb{1} + \omega \mathbb{1} \otimes a^* a + \frac{\lambda}{2} \sigma_z \otimes (a^* + a) \right] \\
&= \frac{\epsilon}{2} P_1 \otimes \mathbb{1} + \omega P_1 \otimes a^* a + \frac{\lambda}{2} P_1 \otimes (a^* + a) \\
&= P_1 \otimes \left( \frac{\epsilon}{2} \mathbb{1} + \omega a^* a + \frac{\lambda}{2} (a^* + a) \right) \\
&= P_1 \otimes H_1
\end{aligned} \tag{2.13}$$

Using (2.7) we have

$$\begin{aligned}
H^2(P_1 \otimes \mathbb{1}) &= H^2(P_1 \otimes \mathbb{1})(P_1 \otimes \mathbb{1}) \\
&= (P_1 \otimes H_1)(P_1 \otimes H_1) \\
&= P_1 \otimes H_1^2.
\end{aligned} \tag{2.14}$$

It follows that

$$H^n(P_1 \otimes \mathbb{1}) = P_1 \otimes H_1^n. \tag{2.15}$$

Using this we obtain

$$\begin{aligned}
(P_1 \otimes \mathbb{1})e^{itH} &= (P_1 \otimes \mathbb{1}) \sum_{n \geq 0} \frac{(it)^n}{n!} H^n \\
&= \sum_{n \geq 0} \frac{(it)^n}{n!} (P_1 \otimes \mathbb{1}) H^n \\
&= \sum_{n \geq 0} \frac{(it)^n}{n!} (P_1 \otimes H_1^n) \\
&= P_1 \otimes \sum_{n \geq 0} \frac{(it)^n}{n!} (H_1^n) \\
&= P_1 \otimes e^{itH_1}.
\end{aligned} \tag{2.16}$$

Similary we have for the projection onto the spin down state  $P_2 = |\downarrow\rangle \langle \downarrow| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$

$$H(P_2 \otimes \mathbb{1}) = P_2 \otimes H_2 \tag{2.17}$$

with

$$H_2 = -\frac{\epsilon}{2} \mathbb{1} + \omega a^* a - \frac{\lambda}{2} (a^* + a) \tag{2.18}$$

being an operator on  $\mathcal{H}_{osc}$ .

As before we get

$$H^n(P_2 \otimes \mathbb{1}) = P_2 \otimes H_2^n \tag{2.19}$$

and also with the same steps as in (2.16) we achieve

$$(P_2 \otimes \mathbb{1})e^{itH} = P_2 \otimes e^{itH_2}. \tag{2.20}$$

Using  $\rho(0) = \sum_{i,j \in \{1,2\}} P_i \rho(0) P_j$ , equations (2.16) and (2.20) and the fact that  $\text{Tr}$  is linear

we can substitute in (2.1)

$$\begin{aligned}
\rho(t) &= \text{Tr}_E(e^{-itH}(\rho(0) \otimes \rho_E)e^{itH}) \\
&= \text{Tr}_E \left( e^{-itH} \sum_{i,j \in \{1,2\}} P_i \rho(0) P_j \otimes \rho_E e^{itH} \right) \\
&= \text{Tr}_E \left( \sum_{i,j \in \{1,2\}} e^{-itH} (P_i \otimes \mathbb{1})(\rho(0) \otimes \rho_E)(P_j \otimes \mathbb{1}) e^{itH} \right) \\
&= \text{Tr}_E \left( \sum_{i,j \in \{1,2\}} (P_i \otimes e^{-itH_i})(\rho(0) \otimes \rho_E)(P_j \otimes e^{itH_j}) \right) \\
&= \sum_{i,j \in \{1,2\}} P_i \rho(0) P_j \text{Tr}_E (e^{-itH_i} \rho_E e^{itH_j}) \\
&= \sum_{i,j \in \{1,2\}} c_{ij} P_i \rho_S(0) P_j,
\end{aligned}$$

which shows (2.10).

For the following Lemma we will define the number operator  $N$  and Field Operator  $\Psi$ .

**Definition 2.1.1.** <sup>1</sup> Let  $z \in \mathbb{C}$ . Then the following are operators on  $\mathcal{H}_{osc}$ . The *number operator*  $N$  and *Field Operator*  $\Psi$  are defined as

$$N = a^* a \tag{2.21}$$

$$\Psi(z) = \frac{za^* + z^*a}{\sqrt{2}}, \quad z \in \mathbb{C}, \tag{2.22}$$

where the ladder operators  $a, a^*$  satisfy the CCR  $[a, a^*] = \mathbb{1}$ . The *Weyl-Operator* is defined as

$$W(z) = e^{i\Psi(z)}. \tag{2.23}$$

**Lemma 2.1.2.** *The following holds for the operators from definition 2.1.1:*

---

<sup>1</sup>We consider bosonic harmonic oscillators in this thesis. From a mathematical view point the creation and annihilation operators are unbounded operators. To circumvent this we introduce the field operator  $\Psi$  and Weyl operator  $W$ . For more detail on this concept and the mathematical rigor see [22].



$$W(z) \text{ is unitary: } W(z)^* = W(-z) = (W(z))^{-1} \quad (2.24)$$

$$CCR: W(z)W(\psi) = e^{-\frac{i}{2} \text{Im}\langle z|\psi \rangle} W(\psi + z) \quad (2.25)$$

$$e^{itN} \Psi(z) e^{-itN} = \Psi(e^{it} z) \quad (2.26)$$

$$e^{itN} W(z) e^{-itN} = W(e^{it} z) \quad (2.27)$$

$$W(z)\Psi(\psi)W(-z) = \Psi(\psi) - \text{Im}\langle z|\psi \rangle \quad (2.28)$$

$$W(z)NW(-z) = N - \Psi(iz) + \frac{|z|^2}{2} \quad (2.29)$$

Note that we here denote the inner product of  $\mathcal{C}$  as  $\langle z|\psi \rangle = z^* \psi$ .

*Proof.* Note that

$$\begin{aligned} (\Psi(z))^* &= \left( \frac{za^* + z^*a}{\sqrt{2}} \right)^* \\ &= \frac{z^*a + za^*}{\sqrt{2}} \\ &= \Psi(z) \end{aligned} \quad (2.30)$$

and  $\Psi(z)$  is a self adjoint real-linear operator.

1.  $W(z)$  is unitary:  $W(z)^* = W(-z) = (W(z))^{-1}$

As  $\Psi(z)$  is self adjoint we have

$$\begin{aligned} W(z)W(-z) &= e^{i\Psi(z)} e^{-i\Psi(z)} \\ &= e^{i(\Psi(z) - \Psi(z))} \\ &= \mathbb{1} \end{aligned}$$

and also

$$\begin{aligned} W(z)^* &= (e^{i\Psi(z)})^* \\ &= e^{(i\Psi(z))^*} \\ &= e^{-i\Psi(z)} \\ &= W(-z). \end{aligned}$$

2. CCR:  $W(z)W(\psi) = e^{-\frac{i}{2} \text{Im}\langle z|\psi \rangle} W(\psi + z)$

We have  $(z^*\psi - z\psi^*) = 2i\text{Im} \langle z|\psi \rangle$ .

$$\begin{aligned}
[\Psi(z), \Psi(\psi)] &= \frac{1}{2}[za^* + z^*a, \psi a^* + \psi^*a] \\
&= \frac{1}{2}(z\psi^*[a^*, a] + z^*\psi[a, a^*]) \quad , \text{ since } [a^*, a^*] = [a, a] = 0 \\
&= \frac{1}{2}(z\psi^*(-\mathbb{1}) + z^*\psi\mathbb{1}) \\
&= i\text{Im} \langle z|\psi \rangle \mathbb{1} \quad , \text{ where } \langle z|\psi \rangle = z^*\psi
\end{aligned} \tag{2.31}$$

Clearly any operator commutes with  $c\mathbb{1}$ , for  $c \in \mathbb{C}$  so  $[[\Psi(z), \Psi(\psi)], \Psi(z)] = 0$  (also for  $\Psi(\psi)$ ) and we can use the Baker-Campbell-Hausdorff formula  $e^A e^B = e^{A+B+\frac{1}{2}[A,B]}$ .

$$\begin{aligned}
W(z)W(\psi) &= e^{i\Psi(z)}e^{i\Psi(\psi)} \\
&= \exp(i\Psi(z) + i\Psi(\psi)) + \frac{1}{2}[i\Psi(z), i\Psi(\psi)] \\
&= \exp\left(i\Psi(z + \psi) - \frac{1}{2}i\text{Im} \langle z|\psi \rangle \mathbb{1}\right) \\
&= W(z + \psi)e^{-\frac{i}{2}\text{Im} \langle z|\psi \rangle}
\end{aligned}$$

$$3. e^{itN}\Psi(z)e^{-itN} = \Psi(e^{it}z)$$

The CCR imply that  $a^*N = (N - \mathbb{1})a^*$  from which we obtain

$$a^*e^{-itN} = e^{-it(N-\mathbb{1})}a^* = e^{-itN}e^{-it}a^* \tag{2.32}$$

and so

$$e^{itN}a^*e^{-itN} = e^{-it}a^*. \tag{2.33}$$

Taking the adjoint gives

$$e^{itN}ae^{itN} = e^{it}a. \tag{2.34}$$

$$4. e^{itN}W(z)e^{-itN} = W(e^{it}z)$$

This follows directly from the proof of (2.26).

$$5. W(z)\Psi(\psi)W(-z) = \Psi(\psi) - \text{Im} \langle z|\psi \rangle$$

As  $[[i\Psi(z), \Psi(\psi)], i\Psi(z)] = [[i\Psi(z), \Psi(\psi)], \Psi(\psi)] = 0$  we can use (A.7)

$$e^X Y e^{-X} = Y + [X, Y] \tag{2.35}$$

and immediately get

$$\begin{aligned} W(z)\Psi(\psi)W(-z) &= e^{i\Psi(z)}\Psi(\psi)e^{-i\Psi(z)} \\ &= \Psi(\psi) - \text{Im} \langle z|\psi \rangle \mathbb{1}. \end{aligned}$$

6.  $W(z)NW(-z) = N - \Psi(iz) + \frac{|z|^2}{2}$

Using (A.7) with  $X = i\Psi(z)$ ,  $Y = N$  and the fact that  $[i\Psi(z), N] = \Psi(-iz)$ ,  $[i\Psi(z), [i\Psi(z), N]] = [i\Psi(z), -\Psi(iz)] = |z|^2$  and  $[X, [X, [X, Y]]] = 0$  we have

$$\begin{aligned} W(z)NW(-z) &= N + [i\Psi(z), N] + \frac{1}{2!}[i\Psi(z), [i\Psi(z), N]] \\ &= N - \Psi(iz) + \frac{1}{2}|z|^2. \end{aligned}$$

■

**Remark 2.1.3.** With Lemma 2.1.2 we calculate

$$\begin{aligned} W(z)e^{it(\omega N + \Psi(\frac{\lambda}{\sqrt{2}}))}W(-z) &= \exp \left[ itW(z) \left( \omega N + \Psi \left( \frac{\lambda}{\sqrt{2}} \right) \right) W(-z) \right] \\ &= \exp \left[ it \left( \omega W(z)NW(-z) + W(z)\Psi \left( \frac{\lambda}{\sqrt{2}} \right) W(-z) \right) \right] \\ &= \exp \left[ it \left( \omega N - \Psi(i\omega z) + \frac{\omega|z|^2}{2} \right. \right. \\ &\quad \left. \left. + \Psi \left( \frac{\lambda}{\sqrt{2}} \right) - \text{Im} \left\langle z \left| \frac{\lambda}{\sqrt{2}} \right\rangle \right) \right]. \end{aligned} \tag{2.36}$$

Similarly we have

$$\begin{aligned} W(z)e^{-it(\omega N - \Psi(\frac{\lambda}{\sqrt{2}}))}W(-z) &= \exp \left[ -it \left( \omega N - \Psi(i\omega z) + \frac{\omega|z|^2}{2} \right. \right. \\ &\quad \left. \left. - \Psi \left( \frac{\lambda}{\sqrt{2}} \right) + \text{Im} \left\langle z \left| \frac{\lambda}{\sqrt{2}} \right\rangle \right) \right] \end{aligned} \tag{2.37}$$

Let  $z_1 = \frac{\lambda}{i\omega\sqrt{2}}$ ,  $z_2 = -\frac{\lambda}{i\omega\sqrt{2}}$  and using remark 2.1.3 we conclude

$$W(z_1)e^{it(\omega N + \Psi(\frac{\lambda}{\sqrt{2}}))}W(-z_1) = e^{it(\omega N - \frac{\lambda^2}{4\omega})} \text{ and} \tag{2.38}$$

$$W(z_2)e^{-it(\omega N - \Psi(\frac{\lambda}{\sqrt{2}}))}W(-z_2) = e^{-it(\omega N - \frac{\lambda^2}{4\omega})}. \tag{2.39}$$

Combining this we can prove the following Lemma:

**Lemma 2.1.4.** *The reduced density matrix  $\rho_S(t)$  for the quantum system of a spin coupled to a single quantum harmonic oscillator governed by the Hamiltonian*

$$H = \frac{\epsilon}{2}\sigma_z + \omega a^*a + \frac{\lambda}{2}\sigma_z \otimes (a^* + a), \quad \lambda, \omega, \epsilon \in \mathbb{R} \quad (2.40)$$

*is given by*

$$\rho_S(t) = \begin{pmatrix} \rho_{11}(0)c_{11} & \rho_{12}(0)c_{12} \\ \rho_{21}(0)c_{21} & \rho_{22}(0)c_{22} \end{pmatrix} \quad (2.41)$$

*with*

$$c_{11} = c_{22} = 1 \quad (2.42)$$

$$c_{21} = e^{it\epsilon} e^{-\frac{1}{2}|\xi|^2 \coth(\beta\omega/2)} \quad (2.43)$$

$$c_{12} = c_{21}^* = e^{-it\epsilon} e^{-\frac{1}{2}|\xi|^2 \coth(\beta\omega/2)} \quad (2.44)$$

$$\xi = \frac{i\lambda}{\omega} (1 - e^{i\omega t}) \quad (2.45)$$

$$|\xi|^2 = \frac{4\lambda^2}{\omega^2} \sin^2\left(\frac{\omega t}{2}\right). \quad (2.46)$$

*Proof.* Let  $i = j$ :

$$\begin{aligned} c_{ii} &= \text{Tr}_E(e^{-itH_i} \rho_E e^{itH_i}) \\ &= \text{Tr}_E(e^{itH_i} e^{-itH_i} \rho_E) \\ &= \text{Tr}_E(\rho_E) \\ &= 1, \end{aligned}$$

as  $\rho_E$  is a density matrix and as such has trace 1.

It follows that

$$c_{11} = c_{22} = 1. \quad (2.47)$$

Now let  $i \neq j$ . For  $z_1 = \frac{\lambda}{i\omega\sqrt{2}}$  and  $z_2 = -\frac{\lambda}{i\omega\sqrt{2}}$  as in (2.38) and (2.39) we have the following

relations for  $z_1$ ,  $z_2$  and  $\lambda$ :

$$z_1 + z_2 = 0 \quad (2.48)$$

$$z_1 - z_2 = \frac{-i\lambda\sqrt{2}}{\omega} \quad (2.49)$$

$$\text{Im} \langle z_1 | z_2 \rangle = 0 \quad (2.50)$$

$$\text{Im} \left\langle z_1 \left| \frac{\lambda}{\sqrt{2}} \right\rangle = \frac{\lambda^2}{2\omega} \quad (2.51)$$

$$\text{Im} \left\langle z_2 \left| \frac{\lambda}{\sqrt{2}} \right\rangle = \frac{-\lambda^2}{2\omega} \quad (2.52)$$

Using this, equations (2.38) , (2.39), Lemma 2.1.2 and the formula (2.8) for  $c_{21}$  we have

$$\begin{aligned} c_{21} &= \text{Tr}_E \left( \rho_E e^{itH_1} e^{-itH_2} \right) \\ &= \text{Tr}_E \left( \rho_E e^{it\left(\epsilon/2 + \omega N + \Psi\left(\frac{\lambda}{\sqrt{2}}\right)\right)} e^{-it\left(-\epsilon/2 + \omega N - \Psi\left(\frac{\lambda}{\sqrt{2}}\right)\right)} \right) \\ &= e^{it\epsilon} \text{Tr}_E \left( \rho_E e^{it\left(\omega N + \Psi\left(\frac{\lambda}{\sqrt{2}}\right)\right)} e^{-it\left(\omega N - \Psi\left(\frac{\lambda}{\sqrt{2}}\right)\right)} \right) \\ &= e^{it\epsilon} \text{Tr}_E \left( \rho_E W(-z_1) W(z_1) e^{it\left(\omega N + \Psi\left(\frac{\lambda}{\sqrt{2}}\right)\right)} W(-z_1) W(z_1) \right. \\ &\quad \left. \times W(-z_2) W(z_2) e^{-it\left(\omega N - \Psi\left(\frac{\lambda}{\sqrt{2}}\right)\right)} W(-z_2) W(z_2) \right) \\ &= e^{it\epsilon} \text{Tr}_E \left( \rho_E W(-z_1) e^{it\left(\omega N - \frac{\lambda^2}{4\omega}\right)} W(z_1) W(-z_2) e^{-it\left(\omega N - \frac{\lambda^2}{4\omega}\right)} W(z_2) \right) \\ &= e^{it\epsilon} \text{Tr}_E \left( \rho_E W(-z_1) e^{it\omega N} e^{-it\frac{\lambda^2}{4\omega}} W(z_1 - z_2) e^{\frac{i}{2}\text{Im}\langle z_1 | z_2 \rangle} e^{-it\omega N} e^{it\frac{\lambda^2}{4\omega}} W(z_2) \right) \\ &= e^{it\epsilon} \text{Tr}_E \left( \rho_E W(-z_1) e^{it\omega N} W(-i\sqrt{2}\lambda/\omega) e^{-it\omega N} W(z_2) \right) \\ &= e^{it\epsilon} \text{Tr}_E \left( \rho_E W(-z_1) W(-e^{i\omega t} i\sqrt{2}\lambda/\omega) W(z_2) \right) \\ &= e^{it\epsilon} \text{Tr}_E \left( \rho_E W(-z_1) W(-e^{i\omega t} i\sqrt{2}\lambda/\omega + z_2) e^{-\frac{i}{2}\text{Im}\langle -e^{i\omega t} i\sqrt{2}\lambda/\omega | z_2 \rangle} \right) \\ &= e^{it\epsilon} \text{Tr}_E \left( \rho_E W(-e^{i\omega t} i\sqrt{2}\lambda/\omega + z_2 - z_1) e^{\frac{i\lambda^2}{2\omega^2} \sin(\omega t)} e^{-\frac{i}{2}\text{Im}\langle -e^{i\omega t} i\sqrt{2}\lambda/\omega + z_2 | -z_1 \rangle} \right) \\ &= e^{it\epsilon} \text{Tr}_E \left( \rho_E W(-e^{i\omega t} i\sqrt{2}\lambda/\omega + i\sqrt{2}\lambda/\omega) e^{-\frac{i\lambda^2}{2\omega^2} \sin(\omega t)} e^{\frac{i\lambda^2}{2\omega^2} \sin(\omega t)} \right) \\ &= e^{it\epsilon} \text{Tr}_E \left( \rho_E W(i\sqrt{2}\lambda(1 - e^{i\omega t})/\omega) \right) \end{aligned}$$

Setting

$$\xi = \frac{i\lambda}{\omega} (1 - e^{i\omega t}) \quad (2.53)$$

we obtain

$$|\xi|^2 = \frac{4\lambda^2}{\omega^2} \sin^2\left(\frac{\omega t}{2}\right) \quad (2.54)$$

and using (2.2) gives

$$\begin{aligned} c_{21} &= e^{it\epsilon} \text{Tr}_E \left( \rho_E W(\xi\sqrt{2}) \right) \\ &= e^{it\epsilon} \text{Tr}_E \left( \rho_E e^{i\Psi(\xi\sqrt{2})} \right) \\ &= e^{it\epsilon} \text{Tr}_E \left( \rho_E e^{i(\xi a^* + \xi^* a)} \right) \\ &= e^{it\epsilon} e^{-\frac{1}{2}|\xi|^2 \coth(\beta\omega/2)}, \end{aligned} \quad (2.55)$$

which is the desired result. Note that since  $c_{ij} = c_{ji}^*$  for density matrices, we have

$$c_{12} = c_{21}^* = e^{-it\epsilon} e^{-\frac{1}{2}|\xi|^2 \coth(\beta\omega/2)}. \quad (2.56)$$

■

## 2.2 Spin coupled to multitude of independent harmonic oscillators

In this section we have a single spin coupled to a multitude of independent quantum harmonic oscillators. The system is governed by the Hamiltonian

$$H = \frac{\epsilon}{2} \sigma_z + \sum_j \omega_j a_j^* a_j + \sum_j \frac{\lambda_j}{2} \sigma_z \otimes (a_j^* + a_j) \quad (2.57)$$

with  $\lambda_j, \omega_j, \epsilon \in \mathbb{R}$  and the commutation relation  $[a_j, a_k^*] = \delta_{jk} \mathbb{1}$ .

We will introduce a bit of notation for ease of use.

**Definition 2.2.1.** We will write

$$\mathbb{1}_j \otimes A \quad (2.58)$$

for

$$\mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes A \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}, \quad (2.59)$$

where the operator  $A$  is at the  $j$ -th position in the tensor product above.

All sums in the following section will run from  $j = 1, \dots, N$ , where  $N$  is a natural number.

Let us take a closer look at the Hilbert Space for the harmonic oscillators. Our Hilbert Space for a multitude of harmonic oscillators is given by  $\mathcal{H}_{osc} = \otimes_j \mathcal{H}_{osc_j}$ , where all  $\mathcal{H}_{osc_j}$  are identical.

The harmonic oscillators are independent, hence they can reach their equilibrium independent of the states of the other oscillators. This means that, if the whole system is in equilibrium, the density matrices are in an untangled state and as such we can write them in the following way

$$\rho_E = \otimes_j \rho_{E_j}, \quad (2.60)$$

where  $\rho_{E_j}$  is the equilibrium state of the  $j$ -th oscillator. For every  $j$ ,  $\rho_{E_j}$  is a density matrix acting on  $\mathcal{H}_{osc_j}$ .

We can now define our number operator  $N_j$  and Field Operator  $\Psi_j(z_j)$  in the Hilbert Space  $\mathcal{H}_{osc_j}$  belonging to the  $j$ -th harmonic oscillator (they are independent!).

In the following section we let  $\vec{\lambda}, \vec{\omega} \in \mathbb{R}^N$ ,  $\vec{z}, \vec{\mu} \in \mathbb{C}^N$  and  $\varphi, \psi$  be arbitrary vectors in  $\mathcal{H}_{osc}$ .

**Definition 2.2.2.** Let  $\mathcal{H}_{osc_j}$  be the Hilbert Space of the  $j$ -th quantum harmonic oscillator in our given system and  $\vec{z} = (z_1, \dots, z_N) \in \mathbb{C}^N$ . Define the  $j$ -th Number Operator  $N_j$  and Field Operator  $\Psi_j$  as

$$N_j : \mathcal{H}_{osc_j} \rightarrow \mathcal{H}_{osc_j} : N_j = a_j^* a_j \quad (2.61)$$

$$\Psi_j : \mathcal{H}_{osc_j} \rightarrow \mathcal{H}_{osc_j} : \Psi_j(z_j) : \frac{z_j^* a_j + z_j a_j^*}{\sqrt{2}}. \quad (2.62)$$

**Definition 2.2.3.** We define the *total number operator*  $N$ , on  $\mathcal{H}_{osc}$  for given  $\vec{\omega}, \vec{z}$ , as

$$N(\vec{\omega}) = \sum_j \mathbb{1}_j \otimes \omega_j N_j \quad (2.63)$$

and the *total Field Operator*  $\Psi$  on  $\mathcal{H}_{osc}$  as

$$\Psi(\vec{z}) = \sum_j \mathbb{1}_j \otimes \Psi_j(z_j). \quad (2.64)$$

**Remark 2.2.4.** We can rewrite the Hamiltonian (2.57)

$$H = \frac{\epsilon}{2} \sigma_z \otimes_j \mathbb{1} + \sum_j \mathbb{1} \otimes \mathbb{1}_j \otimes \omega_j N_j + \sum_j \sigma_z \otimes \mathbb{1}_j \otimes \Psi_j \left( \frac{\lambda_j}{\sqrt{2}} \right) \quad (2.65)$$

$$= \frac{\epsilon}{2} \sigma_z \otimes_j \mathbb{1} + \mathbb{1} \otimes N(\vec{\omega}) + \sigma_z \otimes \Psi \left( \frac{\vec{\lambda}}{\sqrt{2}} \right). \quad (2.66)$$

As before we first prove the claim

$$\rho_S(t) = \sum_{i,j \in \{1,2\}} P_i \rho_S(0) P_j \operatorname{Tr}_E \left( e^{-itH_i} \rho_E e^{itH_j} \right). \quad (2.67)$$

For this we follow the same steps as in section 2.1. Again we need operators  $H_1$  and  $H_2$  such that

$$(P_k \otimes \mathbb{1})H = P_k \otimes H_k \quad \text{for } k = 1, 2. \quad (2.68)$$

We set  $\mathbb{1}_{osc} = \otimes_{j=1}^N \mathbb{1}$ .

$$\begin{aligned} (P_1 \otimes \mathbb{1}_{osc})H &= (P_1 \otimes \mathbb{1}_{osc}) \left( \frac{\epsilon}{2} \sigma_z \otimes \mathbb{1}_{osc} + \mathbb{1} \otimes N(\vec{\omega}) + \sigma_z \otimes \Psi \left( \frac{\vec{\lambda}}{\sqrt{2}} \right) \right) \\ &= \frac{\epsilon}{2} P_1 \otimes \mathbb{1}_{osc} + P_1 \otimes N(\vec{\omega}) + P_1 \otimes \Psi \left( \frac{\vec{\lambda}}{\sqrt{2}} \right) \\ &= P_1 \otimes \left( \frac{\epsilon}{2} + N(\vec{\omega}) + \Psi \left( \frac{\vec{\lambda}}{\sqrt{2}} \right) \right) \\ &= P_1 \otimes H_1 \end{aligned}$$

with

$$H_1 = \frac{\epsilon}{2} + N(\vec{\omega}) + \Psi \left( \frac{\vec{\lambda}}{\sqrt{2}} \right), \quad (2.69)$$

being an operator on  $\mathcal{H}_{osc}$ . Similarly we have for  $H_2$  and  $P_2$

$$(P_2 \otimes \mathbb{1}_{osc})H = P_2 \otimes H_2 \quad (2.70)$$

with

$$H_2 = -\frac{\epsilon}{2} + N(\vec{\omega}) - \Psi \left( \frac{\vec{\lambda}}{\sqrt{2}} \right). \quad (2.71)$$

Using again the fact that

$$(P_k \otimes \mathbb{1}_{osc})H^n = P_k \otimes H_k^n \quad \text{for } k = 1, 2 \quad (2.72)$$



we see with the same steps as in (2.16) that

$$(P_k \otimes \mathbb{1}_{osc})e^{itH} = P_k \otimes e^{itH_k} \quad \text{for } k = 1, 2. \quad (2.73)$$

This proof claims (2.67), with  $H_1, H_2$  given in (2.69) and (2.71).

**Lemma 2.2.5.** *We have the following commutation relations for all  $j, k \in 1, \dots, N$ . Denote by  $\delta_{jk}$  the Kronecker symbol.*

$$[\omega_k N_k, a_j] = -\delta_{jk} \omega_k a_j \quad (2.74)$$

$$[\omega_k N_k, a_j^*] = \delta_{jk} \omega_k a_j^* \quad (2.75)$$

$$[N(\vec{\omega}), a_j^*] = [\omega_j N_j, a_j^*] = \omega_j a_j^* \quad (2.76)$$

$$[N(\vec{\omega}), a_j] = [\omega_j N_j, a_j] = -\omega_j a_j \quad (2.77)$$

$$[N_j, N_k] = 0 \quad (2.78)$$

$$[\Psi(\vec{\mu}), a_j^*] = \frac{\mu_j^*}{\sqrt{2}} \mathbb{1} \quad (2.79)$$

$$[\Psi(\vec{\mu}), a_j] = -\frac{\mu_j}{\sqrt{2}} \mathbb{1} \quad (2.80)$$

$$[\Psi_j(\varphi), \Psi_k(\psi)] = i\delta_{jk} \text{Im} \langle \varphi | \psi \rangle \mathbb{1} \quad (2.81)$$

$$[\Psi(\vec{z}), \Psi(\vec{\mu})] = i \sum_j \text{Im} \langle z_j | \mu_j \rangle \mathbb{1} \quad (2.82)$$

$$[\Psi_k(z_k), \omega_j N_j] = \delta_{jk} \frac{\omega_j}{\sqrt{2}} (z_k^* a_j - z_k a_j^*) \quad (2.83)$$

$$[\Psi(\vec{z}), N(\vec{\omega})] = \sum_j [\Psi_j(z_j), \omega_j N_j] = \sum_j \frac{\omega_j}{\sqrt{2}} (z_j^* a_j - z_j a_j^*) \quad (2.84)$$

*Proof.* All commutation relations are easily obtained through direct computation and the fact that  $[a_j, a_k^*] = \delta_{jk}$ . ■

We can now define the Weyl-Operator.

**Definition 2.2.6.** The  $j$ -th Weyl-Operator on  $\mathcal{H}_{osc_j}$  is defined as

$$W_j(z_j) := e^{i\Psi_j(z_j)} \quad \forall j. \quad (2.85)$$

We define the *total Weyl-Operator* for given  $\vec{z} \in \mathbb{C}^N$  as

$$W(\vec{z}) := \otimes_j W_j(z_j) = \prod_j \mathbb{1}_j \otimes W_j(z_j). \quad (2.86)$$

We will now reproduce Lemma 2.1.2 from the previous section with only one harmonic oscillator for the case of a multitude of oscillators.

**Lemma 2.2.7.** *Let  $\vec{z} = (z_1, \dots, z_N)$  and  $\vec{\mu} = (\mu_1, \dots, \mu_N)$  be vectors in  $\mathbb{C}^N$ . We define*

$$s(\vec{\mu}, \vec{z}) := \sum_j \text{Im} \langle \mu_j | z_j \rangle. \quad (2.87)$$

*For the total number Operator  $N(\vec{\omega})$ , the total Field Operator  $\Psi(\vec{\mu})$  and the total Weyl-Operator  $W(\vec{z})$  we have the following properties*

$$W(\vec{z})^* = W(-\vec{z}) = (W(\vec{z}))^{-1} \quad (2.88)$$

$$W(\vec{z})W(\vec{\mu}) = W(\vec{z} + \vec{\mu})e^{-\frac{i}{2}s(\vec{z}, \vec{\mu})} \quad (2.89)$$

$$e^{itN(\vec{\omega})}\Psi(\vec{z})e^{-itN(\vec{\omega})} = \Psi(e^{it\vec{\omega}}\vec{z}) \quad (2.90)$$

$$e^{itN(\vec{\omega})}W(\vec{z})e^{-itN(\vec{\omega})} = W(e^{it\vec{\omega}}\vec{z}) \quad (2.91)$$

$$W(\vec{z})\Psi(\vec{\mu})W(-\vec{z}) = \Psi(\vec{\mu}) - s(\vec{z}, \vec{\mu}) \quad (2.92)$$

$$W(\vec{z})N(\vec{\omega})W(-\vec{z}) = N(\vec{\omega}) - \Psi(i\vec{\omega}\vec{z}) + \frac{1}{2} \sum_j \omega_j |z_j|^2 \quad (2.93)$$

where by  $\vec{\omega}\vec{z}$  we mean the component wise multiplication of the vectors, i.e.  $\vec{\omega}\vec{z} = (\omega_1 z_1, \omega_2 z_2, \dots)$ .

*Proof.* Clearly again  $\Psi(\vec{z})$  is self adjoint. Note that Lemma 2.1.2 is a special case of this, with  $\mathcal{H}_{osc} = \mathcal{H}_{osc1}$  which we will use here.

$$1. \quad W(\vec{z})^* = W(-\vec{z}) = (W(\vec{z}))^{-1}$$

$$\begin{aligned} W(\vec{z})^* &= (\otimes_j W_j(z_j))^* \\ &= (\otimes_j e^{i\Psi_j(z_j)})^* \\ &= \otimes_j e^{(i\Psi_j(z_j))^*} \\ &= \otimes_j e^{-i\Psi_j(z_j)} \\ &= \otimes_j W_j(-z_j) \\ &= W(-\vec{z}) \end{aligned}$$

and also

$$\begin{aligned}
W(\vec{z})W(-\vec{z}) &= \otimes_j W_j(z_j) \otimes_j W_j(-z_j) \\
&= \otimes_j W_j(z_j)W_j(-z_j) \\
&= \otimes_j e^{i\Psi_j(z_j)} e^{i\Psi_j(-z_j)} \\
&= \otimes_j e^{i(\Psi_j(z_j) - \Psi_j(-z_j))} \\
&= \otimes_j \mathbb{1} = \mathbb{1}_{osc}
\end{aligned}$$

$$2. W(\vec{z})W(\vec{\mu}) = W(\vec{z} + \vec{\mu})e^{-\frac{i}{2}s(\vec{z}, \vec{\mu})}$$

$$\begin{aligned}
W(\vec{z})W(\vec{\mu}) &= \otimes_j W_j(z_j) \otimes_j W_j(\mu_j) \\
&= \otimes_j W_j(z_j)W_j(\mu_j) \\
&= \otimes_j e^{i\Psi_j(z_j + \mu_j) - \frac{i}{2}Im\langle z_j | \mu_j \rangle} \quad (\text{use of Lemma 2.1.2}) \\
&= \left( \prod_j e^{-\frac{i}{2}Im\langle z_j | \mu_j \rangle} \right) \otimes_j e^{i\Psi_j(z_j + \mu_j)} \\
&= e^{-\frac{i}{2}\sum_j Im\langle z_j | \mu_j \rangle} \otimes_j W_j(z_j + \mu_j) \\
&= e^{-\frac{i}{2}s(\vec{z}, \vec{\mu})} W(\vec{z} + \vec{\mu})
\end{aligned}$$

$$3. e^{itN(\vec{\omega})}\Psi(\vec{z})e^{-itN(\vec{\omega})} = \Psi(e^{it\vec{\omega}}\vec{z})$$

$$\begin{aligned}
e^{itN(\vec{\omega})}\Psi(\vec{z})e^{-itN(\vec{\omega})} &= \left( \otimes_j e^{it\omega_j N_j} \right) \left( \sum_j \mathbb{1}_j \otimes \Psi_j(z_j) \right) \left( \otimes_j e^{-it\omega_j N_j} \right) \\
&= \sum_j \left[ \left( \otimes_j e^{it\omega_j N_j} \right) \left( \mathbb{1}_j \otimes \Psi_j(z_j) \right) \left( \otimes_j e^{-it\omega_j N_j} \right) \right] \\
&= \sum_j \left[ \mathbb{1}_j \otimes e^{it\omega_j N_j} \Psi_j(z_j) e^{-it\omega_j N_j} \right] \\
&= \sum_j \left[ \mathbb{1}_j \otimes \Psi_j(e^{it\omega_j} z_j) \right] \quad (\text{use of Lemma 2.1.2}) \\
&= \Psi(e^{it\vec{\omega}} \vec{z})
\end{aligned}$$

$$4. e^{itN(\vec{\omega})}W(\vec{z})e^{-itN(\vec{\omega})} = W(e^{it\vec{\omega}}\vec{z})$$

$$\begin{aligned}
e^{itN(\vec{\omega})}W(\vec{z})e^{-itN(\vec{\omega})} &= \left(e^{it\sum_j \mathbb{1}_j \otimes \omega_j N_j}\right) \left(\otimes_j W_j(z_j)\right) \left(e^{-it\sum_j \mathbb{1}_j \otimes \omega_j N_j}\right) \\
&= \left(\prod_j \mathbb{1}_j \otimes e^{it\omega_j N_j}\right) \left(\otimes_j W_j(z_j)\right) \left(\prod_j \mathbb{1}_j \otimes e^{-it\omega_j N_j}\right) \\
&= (\otimes_j e^{it\omega_j N_j}) (\otimes_j W_j(z_j)) (\otimes_j e^{-it\omega_j N_j}) \\
&= \otimes_j e^{it\omega_j N_j} W_j(z_j) e^{-it\omega_j N_j} \\
&= \otimes_j W_j(e^{it\omega_j} z_j) \quad (\text{use of Lemma 2.1.2}) \\
&= W(e^{it\vec{\omega}} \vec{z})
\end{aligned}$$

$$5. W(\vec{z})\Psi(\vec{\mu})W(-\vec{z}) = \Psi(\vec{\mu}) - s(\vec{z}, \vec{\mu})$$

$$\begin{aligned}
W(\vec{z})\Psi(\vec{\mu})W(-\vec{z}) &= \left(\otimes_j W_j(z_j)\right) \left(\sum_j \mathbb{1}_j \otimes \Psi_j(\mu_j)\right) \left(\otimes_j W_j(-z_j)\right) \\
&= \sum_j \left[\mathbb{1}_j \otimes W_j(z_j)\Psi_j(\mu_j)W_j(-z_j)\right] \\
&= \sum_j \left[\mathbb{1}_j \otimes (\Psi_j(\mu_j) - Im\langle z_j | \mu_j \rangle)\right] \quad (\text{use of Lemma 2.1.2}) \\
&= \sum_j \mathbb{1}_j \otimes \Psi_j(\mu_j) - \sum_j Im\langle z_j | \mu_j \rangle \\
&= \Psi(\vec{\mu}) - s(\vec{z}, \vec{\mu}) \mathbb{1}_{osc}
\end{aligned}$$

$$6. W(\vec{z})N(\vec{\omega})W(-\vec{z}) = N(\vec{\omega}) - \Psi(i\vec{\omega}\vec{z}) + \frac{1}{2} \sum_j \omega_j |z_j|^2$$

$$\begin{aligned}
W(\vec{z})N(\vec{\omega})W(-\vec{z}) &= \left(\otimes_j W_j(z_j)\right) \left(\sum_j \mathbb{1}_j \otimes \omega_j N_j\right) \left(\otimes_j W_j(-z_j)\right) \\
&= \sum_j \left[\mathbb{1}_j \otimes W_j(z_j)\omega_j N_j W_j(-z_j)\right] \\
&= \sum_j \left[\mathbb{1}_j \otimes \left(\omega_j N_j - \Psi_j(i\omega_j z_j) + \frac{\omega_j |z_j|^2}{2}\right)\right] \quad (\text{use of Lemma 2.1.2}) \\
&= \sum_j \mathbb{1}_j \otimes \omega_j N_j - \sum_j \mathbb{1}_j \otimes \Psi_j(i\omega_j z_j) + \sum_j \mathbb{1}_j \otimes \frac{\omega_j |z_j|^2}{2} \\
&= N(\vec{\omega}) - \Psi(i\vec{\omega}\vec{z}) + \sum_j \frac{\omega_j |z_j|^2}{2} \mathbb{1}_{osc}
\end{aligned}$$

■

**Remark 2.2.8.** With Lemma 2.2.7 we calculate for  $\vec{z} \in \mathbb{C}^N$ ,  $\vec{\lambda}, \vec{\omega} \in \mathbb{R}^N$

$$\begin{aligned}
W(\vec{z})e^{it(N(\vec{\omega})+\Psi(\frac{\vec{\lambda}}{\sqrt{2}}))}W(-\vec{z}) &= \exp \left[ it \left( W(\vec{z})N(\vec{\omega})W(-\vec{z}) \right. \right. \\
&\quad \left. \left. + W(\vec{z})\Psi\left(\frac{\vec{\lambda}}{\sqrt{2}}\right)W(-\vec{z}) \right) \right] \\
&= \exp \left[ it \left( N(\vec{\omega}) - \Psi(i\vec{\omega}\vec{z}) + \frac{1}{2} \sum_j \omega_j |z_j|^2 \right. \right. \\
&\quad \left. \left. + \Psi\left(\frac{\vec{\lambda}}{\sqrt{2}}\right) - s(\vec{z}, \vec{\lambda}/\sqrt{2}) \right) \right]
\end{aligned} \tag{2.94}$$

and also

$$\begin{aligned}
W(\vec{z})e^{it(N(\vec{\omega})-\Psi(\frac{\vec{\lambda}}{\sqrt{2}}))}W(-\vec{z}) &= \exp \left[ it \left( W(\vec{z})N(\vec{\omega})W(-\vec{z}) - W(\vec{z})\Psi\left(\frac{\vec{\lambda}}{\sqrt{2}}\right)W(-\vec{z}) \right) \right] \\
&= \exp \left[ it \left( N(\vec{\omega}) - \Psi(i\vec{\omega}\vec{z}) + \frac{1}{2} \sum_j \omega_j |z_j|^2 \right. \right. \\
&\quad \left. \left. - \Psi\left(\frac{\vec{\lambda}}{\sqrt{2}}\right) + s(\vec{z}, \vec{\lambda}/\sqrt{2}) \right) \right].
\end{aligned} \tag{2.95}$$

Let  $\vec{z}_1 = \frac{-i\vec{\lambda}}{\vec{\omega}\sqrt{2}}$ ,  $\vec{z}_2 = \frac{i\vec{\lambda}}{\vec{\omega}\sqrt{2}}$ , where  $\frac{\vec{\lambda}}{\vec{\omega}}$  is the component wise division. We calculate

$$s\left(\vec{z}_1, \frac{\vec{\lambda}}{\sqrt{2}}\right) = \sum_j \frac{\lambda_j^2}{2\omega_j} \tag{2.96}$$

$$s\left(\vec{z}_2, \frac{\vec{\lambda}}{\sqrt{2}}\right) = - \sum_j \frac{\lambda_j^2}{2\omega_j} \tag{2.97}$$

and conclude

$$W(\vec{z}_1)e^{it(N(\vec{\omega})+\Psi(\frac{\vec{\lambda}}{\sqrt{2}}))}W(-\vec{z}_1) = e^{it(N(\vec{\omega})-\frac{1}{4}\sum_j \frac{\lambda_j^2}{\omega_j})} \tag{2.98}$$

$$W(\vec{z}_2)e^{it(N(\vec{\omega})-\Psi(\frac{\vec{\lambda}}{\sqrt{2}}))}W(-\vec{z}_2) = e^{it(N(\vec{\omega})-\frac{1}{4}\sum_j \frac{\lambda_j^2}{\omega_j})}. \tag{2.99}$$

We now calculate the density matrix  $\rho_S(t)$  with the following Lemma.

**Lemma 2.2.9.** *The reduced density matrix  $\rho_S(t)$  for the Hamiltonian*

$$H = \frac{\epsilon}{2} \sigma_z \otimes \mathbb{1}_{osc} + \mathbb{1} \otimes N(\vec{\omega}) + \sigma_z \otimes \Psi\left(\frac{\vec{\lambda}}{\sqrt{2}}\right) \quad (2.100)$$

*is given by*

$$\rho_S(t) = \begin{pmatrix} \rho_{11}(0)c_{11} & \rho_{12}(0)c_{12} \\ \rho_{21}(0)c_{21} & \rho_{22}(0)c_{22} \end{pmatrix} \quad (2.101)$$

*with*

$$c_{11} = c_{22} = 1 \quad (2.102)$$

$$c_{21} = e^{it\epsilon} e^{-\frac{1}{2} \sum_j |\xi_j|^2 \coth\left(\frac{\beta\omega_j}{2}\right)} \quad (2.103)$$

$$c_{12} = (c_{21})^* \quad (2.104)$$

$$\xi_j = \frac{i\lambda_j}{\omega_j} (1 - e^{it\omega_j}). \quad (2.105)$$

*Proof.* Let  $i = j$ :

$$\begin{aligned} c_{ii} &= \text{Tr}_E(e^{-itH_i} \rho_E e^{itH_i}) \\ &= \text{Tr}_E(e^{itH_i} e^{-itH_i} \rho_E) \\ &= \text{Tr}_E(\rho_E) \\ &= \text{Tr}_E(\otimes_j \rho_{E_j}) \\ &= \prod_j \text{Tr}_E(\rho_{E_j}) \\ &= 1 \end{aligned}$$

as  $\rho_{E_j}$  is a density matrix for all  $j$  and as such has trace 1.

$$\Rightarrow c_{11} = c_{22} = 1 \quad (2.106)$$

Now let  $i \neq j$ . Choosing  $\vec{z}_1$  and  $\vec{z}_2$  as in (2.98) and (2.99) we have the following relations

for  $\vec{z}_1$  and  $\vec{z}_2$ :

$$\vec{z}_1 = (\vec{z}_2)^* \quad (2.107)$$

$$\vec{z}_1 - \vec{z}_2 = -\frac{i\sqrt{2}\vec{\lambda}}{\vec{\omega}} \quad (2.108)$$

$$s(\vec{z}_1, \vec{z}_2) = 0 \quad (2.109)$$

Calculating  $c_{21}$  with (2.8):

$$\begin{aligned}
c_{21} &= \text{Tr}_E \left( \rho_E e^{itH_1} e^{-itH_2} \right) \\
&= \text{Tr}_E \left( \rho_E e^{it(\frac{\epsilon}{2} + N(\vec{\omega}) + \Psi(\frac{\vec{\lambda}}{\sqrt{2}}))} e^{-it(-\frac{\epsilon}{2} + N(\vec{\omega}) - \Psi(\frac{\vec{\lambda}}{\sqrt{2}}))} \right) \\
&= e^{it\epsilon} \text{Tr}_E \left( \rho_E e^{it(N(\vec{\omega}) + \Psi(\frac{\vec{\lambda}}{\sqrt{2}}))} e^{-it(N(\vec{\omega}) - \Psi(\frac{\vec{\lambda}}{\sqrt{2}}))} \right) \\
&= e^{it\epsilon} \text{Tr}_E \left( \rho_E W(-\vec{z}_1) W(\vec{z}_1) e^{it(N(\vec{\omega}) + \Psi(\frac{\vec{\lambda}}{\sqrt{2}}))} W(-\vec{z}_1) W(\vec{z}_1) \right. \\
&\quad \left. \times W(-\vec{z}_2) W(\vec{z}_2) e^{-it(N(\vec{\omega}) - \Psi(\frac{\vec{\lambda}}{\sqrt{2}}))} W(-\vec{z}_2) W(\vec{z}_2) \right) \\
&= e^{it\epsilon} \text{Tr}_E \left( \rho_E W(-\vec{z}_1) e^{it(N(\vec{\omega}) - \frac{1}{4} \sum_j \frac{\lambda_j^2}{\omega_j^2})} W(\vec{z}_1) W(-\vec{z}_2) e^{-it(N(\vec{\omega}) - \frac{1}{4} \sum_j \frac{\lambda_j^2}{\omega_j^2})} W(\vec{z}_2) \right) \\
&= e^{it\epsilon} \text{Tr}_E \rho_E \left( W(-\vec{z}_1) e^{itN(\vec{\omega})} W(\vec{z}_1 - \vec{z}_2) e^{-\frac{i}{2}s(\vec{z}_1, -\vec{z}_2)} e^{-itN(\vec{\omega})} W(\vec{z}_2) \right) \\
&= e^{it\epsilon} \text{Tr}_E \rho_E \left( W(-\vec{z}_1) e^{itN(\vec{\omega})} W(-\frac{i\sqrt{2}\vec{\lambda}}{\vec{\omega}}) e^{-itN(\vec{\omega})} W(\vec{z}_2) \right) \\
&= e^{it\epsilon} \text{Tr}_E \rho_E \left( W(-\vec{z}_1) W(-e^{it\vec{\omega}} \frac{i\sqrt{2}\vec{\lambda}}{\vec{\omega}}) W(\vec{z}_2) \right) \\
&= e^{it\epsilon} \text{Tr}_E \left( \rho_E W(-\vec{z}_1) W(-e^{it\vec{\omega}} \frac{i\sqrt{2}\vec{\lambda}}{\vec{\omega}} + \vec{z}_2) e^{-\frac{i}{2} \sum_j \frac{\lambda_j^2}{\omega_j^2} \sin(\omega_j t)} \right) \\
&= e^{it\epsilon} \text{Tr}_E \left( \rho_E W(-e^{it\vec{\omega}} \frac{i\sqrt{2}\vec{\lambda}}{\vec{\omega}} + \vec{z}_2 - \vec{z}_1) e^{-\frac{i}{2} \sum_j \frac{\lambda_j^2}{\omega_j^2} \sin(\omega_j t)} e^{\frac{i}{2} \sum_j \frac{\lambda_j^2}{\omega_j^2} \sin(\omega_j t)} \right) \\
&= e^{it\epsilon} \text{Tr}_E \left( \rho_E W \left( \frac{i\sqrt{2}\vec{\lambda}}{\vec{\omega}} (1 - e^{it\vec{\omega}}) \right) \right)
\end{aligned}$$

Set

$$\vec{\xi} = \frac{i\vec{\lambda}}{\vec{\omega}}(1 - e^{it\vec{\omega}}) \quad (2.110)$$

$$\implies |\xi_j|^2 = \frac{4\lambda_j^2}{\omega_j^2} \sin^2\left(\frac{\omega_j t}{2}\right). \quad (2.111)$$

Using this we obtain the desired result

$$\begin{aligned} c_{21} &= e^{it\epsilon} \text{Tr}_E(\rho_E W(\vec{\xi}\sqrt{2})) \\ &= e^{it\epsilon} \text{Tr}_E(\otimes_j \rho_{E_j} \otimes_j W_j(\xi_j\sqrt{2})) \\ &= e^{it\epsilon} \text{Tr}_E(\otimes_j \rho_{E_j} W_j(\xi_j\sqrt{2})) \\ &= e^{it\epsilon} \prod_j \text{Tr}_{E_j}(\rho_{E_j} W_j(\xi_j\sqrt{2})) \\ &= e^{it\epsilon} \prod_j e^{-\frac{1}{2}|\xi_j|^2 \coth\left(\frac{\beta\omega_j}{2}\right)} \\ &= e^{it\epsilon} e^{-\frac{1}{2}\sum_j |\xi_j|^2 \coth\left(\frac{\beta\omega_j}{2}\right)}. \end{aligned}$$

Again we have

$$c_{12} = c_{21}^* = e^{-it\epsilon} e^{-\frac{1}{2}\sum_j |\xi_j|^2 \coth\left(\frac{\beta\omega_j}{2}\right)}. \quad (2.112)$$

■

Note that we could also replace in (2.103)  $\beta$  by  $\beta_j$ , if each oscillator is taken at its own temperature  $\frac{1}{\beta_j}$ .

## 2.3 Spin coupled to free bosonic quantum field

Here we have a spin coupled to a free bosonic field which is governed by the Hamiltonian

$$H = \frac{\epsilon}{2}\sigma_z + H_E + \frac{\lambda}{2}\sigma_z \otimes \Psi(g), \quad (2.113)$$

where

$$H_E = \int_{\mathbb{R}^3} \omega(k) a^*(k) a(k) d^3k, \quad \Psi(g) = \int_{\mathbb{R}^3} (g(k) a^*(k) + \bar{g}(k) a(k)) d^3k. \quad (2.114)$$



The annihilation and creation operators,  $a(k)$  and  $a^*(k)$ , obey the CCR  $[a(k), a^*(l)] = \delta(k - l)$ . The number operator is  $N = \int_{\mathbb{R}^3} a^*(k)a(k)d^3k$ ,  $\frac{\lambda}{2}$  is the coupling factor and  $g(k)$  is a form factor for  $g \in L^2(\mathbb{R}^3, d^3k)$ . The spin interacts with the free bosonic field through the interaction Hamiltonian

$$H_I = \frac{\lambda}{2}\sigma_z \otimes \Psi(g). \quad (2.115)$$

The free Hamiltonian of the reservoir is given by  $H_E$ . We mathematically model a free quantum bosonic field as an infinite system of coupled quantum harmonic oscillators at every space point. We can simply perform an infinite-volume limit for the model in section 2.2 and make the following changes to this model

$$\begin{aligned} \sum_j &\rightarrow \int_{\mathbb{R}^3} d^3k \\ \omega_j &\rightarrow \omega(k) \\ \lambda_j &\rightarrow g(k) \end{aligned}$$

Now define the functions  $\gamma(t)$  and  $\Gamma(t)$  as follows:

$$\Gamma(t) = \int_{\mathbb{R}^3} \frac{|g(k)|^2}{\omega^2(k)} \frac{1 - \cos(\omega(k)t)}{2} \coth\left(\frac{\omega(k)\beta}{2}\right) d^3k \quad (2.116)$$

$$\frac{d\Gamma(t)}{dt} = \gamma(t) = \frac{1}{2} \int_{\mathbb{R}^3} \frac{|g(k)|^2}{\omega(k)} \sin(\omega(k)t) \coth\left(\frac{\omega(k)\beta}{2}\right) d^3k \quad (2.117)$$

Using the spectral density function  $J(\omega) = \frac{\pi}{2}\omega^2 \int_{S^2} |g(k)|^2 d\Sigma$  from section B we can rewrite  $\Gamma(t)$  and  $\gamma(t)$  as

$$\Gamma(t) = \frac{1}{\pi} \int_0^\infty J(\omega) \frac{1 - \cos(\omega t)}{\omega^2} \coth\left(\frac{\beta\omega}{2}\right) d\omega \quad (2.118)$$

$$\gamma(t) = \frac{1}{\pi} \int_0^\infty J(\omega) \frac{\sin \omega t}{\omega} \coth\left(\frac{\beta\omega}{2}\right) d\omega. \quad (2.119)$$

Thus we have for the evolution of the density matrix  $\rho_S(t)$  of the spin under the Hamiltonian (2.113)

$$\rho_S(t) = \begin{pmatrix} \rho_{11}(0)c_{11} & \rho_{12}(0)c_{12} \\ \rho_{21}(0)c_{21} & \rho_{22}(0)c_{22} \end{pmatrix} \quad (2.120)$$

with

$$c_{11} = c_{22} = 1 \quad (2.121)$$

$$c_{21} = e^{it\epsilon} e^{-\lambda^2 \Gamma(t)} \quad (2.122)$$

$$c_{12} = c_{21}^*. \quad (2.123)$$

## Summary

In chapter 2 we considered a spin coupled to a

- single quantum harmonic oscillator mode
- multitude of quantum harmonic oscillators
- free bosonic field

in this chapter. Using (see (2.1))

$$\rho_S(t) = \text{Tr}_E(e^{-itH}(\rho_S(0) \otimes \rho_E)e^{itH}), \quad (2.124)$$

we calculated the explicit reduced density matrix  $\rho_S(t)$  of the spin (see (Lemmas 2.1.4, 2.2.9 and equation (2.120) and following), for the given Hamiltonian  $H$  in each case. For example the density matrix  $\rho_S(t)$  of the spin coupled to the free bosonic field is given by

$$\rho_S(t) = \begin{pmatrix} \rho_{11}(0) & e^{-it\epsilon} e^{-\lambda^2 \Gamma(t)} \\ \rho_{21}(0) e^{it\epsilon} e^{-\lambda^2 \Gamma(t)} & \rho_{22}(0) \end{pmatrix}, \quad (2.125)$$

with  $\Gamma(t)$  given by (2.118). The explicit form of the reduced spin density matrix will be used in the next chapter to analyze the non-Markovianity.

# Chapter 3

## Calculation of non-Markovianity

In this chapter we will calculate explicitly the non-Markovianity  $N(\Phi)$  for the quantum systems of chapter 2. Recall the definition of the non-Markovianity

$$N(\Phi) = \max_{\rho(0), \nu(0)} \int_{\sigma > 0} \sigma(t, \rho, \nu) dt \quad (3.1)$$

based on the increase of the trace distance  $D(t, \rho(t), \nu(t))$  of two initial quantum states  $\rho(0)$  and  $\nu(0)$ . To explicitly calculate  $N(\Phi)$  we need to specify the initial states  $\rho(0)$  and  $\nu(0)$ . We will see in the following chapter that  $N(\Phi)$  can be a finite number as well as infinite.

### 3.1 Spin coupled to single harmonic oscillator

Recalling the calculations from section 2.1 with Hamiltonian

$$H = \frac{\epsilon}{2} \sigma_z + \omega a^* a + \frac{\lambda}{2} \sigma_z \otimes (a^* + a) \quad \lambda, \omega, \epsilon \in \mathbb{R} \quad (3.2)$$

we found the reduced density matrix  $\rho_S(t)$  of the spin to be given by

$$\rho_S(t) = \begin{pmatrix} \rho_{11}(0) & c_{21}^* \rho_{12}(0) \\ c_{21} \rho_{21}(0) & \rho_{22}(0) \end{pmatrix} \quad (3.3)$$

with

$$c_{21}(t) = e^{it\epsilon} e^{-\frac{2\lambda^2}{\omega^2} \sin^2\left(\frac{\omega t}{2}\right) \coth\left(\frac{\beta\omega}{2}\right)}. \quad (3.4)$$

Now let us consider two arbitrary initial spin states  $\rho(0)$  and  $\nu(0)$  (we drop the subscript  $S$  for the system here). The general density matrices  $\rho(t)$  and  $\nu(t)$  for  $t \geq 0$  are given by

$$\rho(t) = \begin{pmatrix} \rho_{11}(0) & \rho_{12}(0)c_{12} \\ \rho_{12}^*(0)c_{12}^* & 1 - \rho_{11}(0) \end{pmatrix} \quad (3.5)$$

$$\nu(t) = \begin{pmatrix} \nu_{11}(0) & \nu_{12}(0)c_{12} \\ \nu_{12}^*(0)c_{12}^* & 1 - \nu_{11}(0) \end{pmatrix} \quad (3.6)$$

Note that  $c_{12} = c_{12}(t)$  and depends on the time  $t$ . Recall the trace distance for a qubit system from Lemma 1.2.3

$$D(t, \rho, \nu) = \sqrt{\alpha^2 + |v(t)|^2} \quad (3.7)$$

with

$$\alpha(t) = \rho_{11}(0) - \nu_{11}(0) \quad (3.8)$$

$$v(t) = \rho_{12}(0)c_{12}(t) - \nu_{12}(0)c_{12}(t) = (\rho_{12}(0) - \nu_{12}(0))c_{12}(t) =: bc_{12}(t) \quad (3.9)$$

$$|v(t)|^2 = |b|^2 |c_{12}(t)|^2 = |b|^2 e^{-\frac{4\lambda^2}{\omega^2} \sin^2(\frac{\omega t}{2}) \coth(\frac{\beta\omega}{2})}. \quad (3.10)$$

Calculating the rate of change  $\sigma(t, \rho, \nu)$  of the trace distance with equation (1.44),  $2 \sin(a) \cos(a) = \sin(2a)$  and

$$\begin{aligned} \text{Re}(v'(t)v^*(t)) &= \frac{1}{2} \partial_t |v(t)|^2 = -|b|^2 \exp\left(-\frac{4\lambda^2}{\omega^2} \sin^2\left(\frac{\omega t}{2}\right) \times \right. \\ &\quad \left. \coth\left(\frac{\beta\omega}{2}\right)\right) \coth(\beta\omega/2) \frac{-4\lambda^2}{\omega^2} \left\{ 2 \frac{\omega}{2} \sin\left(\frac{\omega t}{2}\right) \cos\left(\frac{\omega t}{2}\right) \right\} \\ &= -\frac{\lambda^2}{\omega} \sin(\omega t) \coth\left(\frac{\beta\omega}{2}\right) |v(t)|^2 \end{aligned} \quad (3.11)$$

yields

$$\sigma(t, \rho, \nu) = \frac{-\lambda^2 \sin(\omega t) \coth(\frac{\beta\omega}{2}) |v(t)|^2}{\omega \sqrt{\alpha^2 + |v(t)|^2}}. \quad (3.12)$$

Set

$$K(t) = \frac{2\lambda^2}{\omega^2} \sin^2\left(\frac{\omega t}{2}\right) \coth\left(\frac{\beta\omega}{2}\right) \quad (3.13)$$

$$\Rightarrow \frac{d}{dt} K(t) = \kappa(t) = \frac{\lambda^2}{\omega} \sin(\omega t) \coth\left(\frac{\beta\omega}{2}\right) \quad (3.14)$$

Then  $|v(t)|^2 = |b|^2 e^{-2K(t)}$  and

$$\sigma(t, \rho, \nu) = \frac{-\kappa(t)|b|^2 e^{-2K(t)}}{\sqrt{\alpha^2 + |b|^2 e^{-2K(t)}}}. \quad (3.15)$$

Here one can already see that for a non-Markovian process,  $\sigma > 0$ , we must have  $\kappa(t) < 0$ , provided  $b \neq 0$ .

We can write now

$$\begin{aligned} N(\Phi) &= \max_{\rho(0), \nu(0)} \int_{\sigma > 0} \sigma(t, \rho(0), \nu(0)) dt \\ &= \max_{\alpha, b} \int_{\kappa(t) < 0} \frac{-\kappa(t)|b|^2 e^{-2K(t)}}{\sqrt{\alpha^2 + |b|^2 e^{-2K(t)}}} dt \end{aligned} \quad (3.16)$$

and to maximize the above equation we recall that

$$\sqrt{\alpha^2 + |b|^2 e^{-2K(t)}} = D(t, \rho, \nu)$$

with  $0 \leq D \leq 1$  (see Remark 1.1.8.). Thus since  $e^{-2\Gamma(t)} \in (0, 1]$ ,  $\forall t \in [0, \infty)$ , we must have  $|b|^2 \in (0, 1]$ . It then follows that  $\alpha^2 \in [0, 1)$ . We can now maximize equation (3.16) with the restrictions

$$\alpha^2 \in [0, 1) \quad \text{and} \quad |b|^2 \in (0, 1]. \quad (3.17)$$

Clearly for fixed  $b \in (0, 1]$  the function

$$g(\alpha) = \frac{\kappa(t)|b|^2 e^{-2K(t)}}{\sqrt{\alpha^2 + |b|^2 e^{-2K(t)}}} \quad (3.18)$$

is decreasing for  $\alpha^2 \rightarrow 1$ . Hence  $g(\alpha)$  takes its maximum at  $\alpha = 0$ .

Also for fixed  $\alpha^2 \in [0, 1)$  the function

$$h(b) = \frac{\kappa(t)|b|^2 e^{-2K(t)}}{\sqrt{\alpha^2 + |b|^2 e^{-2K(t)}}} \quad (3.19)$$

is increasing for  $|b|^2 \rightarrow 1$  and thus takes its maximum at  $|b|^2 = 1$ .

It then follows that equation (3.16) maximizes for  $\alpha = 0$  and  $|b|^2 = 1$ . Thus we have

$$\begin{aligned}
N(\Phi) &= \max_{\alpha, b} \int_{\kappa(t) < 0} \frac{-\kappa(t) |b|^2 e^{-2K(t)}}{\sqrt{\alpha^2 + |b|^2 e^{-2K(t)}}} dt \\
&= \int_{\kappa(t) < 0} \frac{-\kappa(t) e^{-2K(t)}}{\sqrt{e^{-2K(t)}}} dt \\
&= \int_{\kappa(t) < 0} -\kappa(t) e^{-K(t)} dt \\
&= \sum_{k \geq 1} e^{-K(b_k)} - e^{-K(a_k)}.
\end{aligned} \tag{3.20}$$

Here  $(a_k, b_k)$  are the time intervals in  $(0, \infty]$  for which we have  $\kappa(t) < 0$ . Clearly (recall  $\omega > 0$ )

$$\kappa(t) = \frac{\lambda^2}{\omega} \sin(\omega t) \coth\left(\frac{\beta\omega}{2}\right) < 0 \Leftrightarrow \sin(\omega t) < 0 \tag{3.21}$$

$$\Leftrightarrow t \in \left(\frac{(2k-1)\pi}{\omega}, \frac{2k\pi}{\omega}\right), k \in \mathbb{Z}. \tag{3.22}$$

Thus

$$(a_k, b_k) = \left(\frac{\pi}{\omega}(2k-1), \frac{2\pi}{\omega}k\right) \text{ for } k \in \mathbb{N}. \tag{3.23}$$

Choosing any two initial states  $\rho, \nu$  that satisfy  $\rho_{11}(0) - \nu_{11}(0) = \alpha = 0$  and  $|\rho_{12}(0) - \nu_{12}(0)|^2 = |b|^2 = 1$  as initial states lets us calculate the non-markovianity. Let

$$|\Theta\rangle := \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle) \tag{3.24}$$

$$|\chi\rangle := \frac{1}{\sqrt{2}}(|+\rangle - |-\rangle), \tag{3.25}$$

which gives the density matrices

$$\rho(0) = |\Theta\rangle \langle \Theta| = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \tag{3.26}$$

$$\nu(0) = |\chi\rangle \langle \chi| = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \tag{3.27}$$

as initial states. They clearly satisfy

$$\alpha = \rho_{11}(0) - \nu_{11}(0) = 1 - 1 = 0 \quad (3.28)$$

$$b = \rho_{12}(0) - \nu_{12}(0) = \frac{1}{2} + \frac{1}{2} = 1. \quad (3.29)$$

With

$$K(b_k) = K\left(\frac{2k\pi}{\omega}\right) = 0 \quad (3.30)$$

$$K(a_k) = K\left(\frac{(2k-1)\pi}{\omega}\right) = \frac{2\lambda^2}{\omega^2} \coth\left(\frac{\beta\omega}{2}\right) \quad (3.31)$$

we can calculate

$$\begin{aligned} N(\Phi) &= \sum_{k \in \mathbb{N}} e^{-K(b_k)} - e^{-K(a_k)} \\ &= \sum_{k \in \mathbb{N}} \left( 1 - e^{-\frac{2\lambda^2}{\omega^2} \coth\left(\frac{\beta\omega}{2}\right)} \right) \\ &= \infty, \quad \text{as } \coth\left(\frac{\beta\omega}{2}\right) > 0. \end{aligned} \quad (3.32)$$

Here we have thus given a non-Markovian process for which we have an infinite amount of non-markovianity. This means that we can never approximate the quantum system, spin coupled to one quantum harmonic oscillator, with a Markovian master equation.

## 3.2 Spin coupled to multitude of independent harmonic oscillators

Here we have a spin coupled to a multitude (finite number) of independent harmonic oscillators. This system is represented by the Hamiltonian

$$H = \frac{\epsilon}{2} \sigma_z \otimes_j \mathbb{1} + \mathbb{1} \otimes N(\vec{\omega}) + \sigma_z \otimes \Phi\left(\frac{\vec{\lambda}}{\sqrt{2}}\right). \quad (3.33)$$

In section 2.2 we calculated the density matrix governing the time evolution to be (again we drop the subscript  $S$  from here on)

$$\rho(t) = \begin{pmatrix} \rho_{11}(0) & \rho_{12}(0)c_{21}^* \\ \rho_{21}(0)c_{21} & \rho_{22}(0) \end{pmatrix} \quad (3.34)$$

with

$$c_{21} = e^{it\epsilon} e^{-\frac{1}{2} \sum_j |\xi_j|^2 \coth\left(\frac{\beta\omega_j}{2}\right)} \quad (3.35)$$

$$|\xi_j|^2 = 4 \frac{\lambda_j^2}{\omega_j^2} \sin^2\left(\frac{\omega_j t}{2}\right). \quad (3.36)$$

Following the same route as in the previous section we will calculate the non-Markovianity and note that we have given finite sums here. The trace distance for two initial states  $\rho(0)$  and  $\nu(0)$ , according to Lemma 1.2.3, is given by

$$D(t, \rho, \nu) = \sqrt{\alpha(t)^2 + |v(t)|^2} \quad (3.37)$$

with

$$\alpha(t) = \rho_{11}(0) - \nu_{11}(0) \quad (3.38)$$

$$v(t) = \rho_{12}(0)c_{12}(t) - \nu_{12}(0)c_{12}(t) = (\rho_{12}(0) - \nu_{12}(0))c_{12}(t) =: v c_{12}(t) \quad (3.39)$$

$$|v(t)|^2 = |v|^2 |c_{12}(t)|^2 = |v|^2 e^{-4 \sum_j \frac{\lambda_j^2}{\omega_j^2} \sin^2\left(\frac{\omega_j t}{2}\right) \coth\left(\frac{\beta\omega_j}{2}\right)}. \quad (3.40)$$

Setting

$$\Gamma(t) = 2 \sum_j \frac{\lambda_j^2}{\omega_j^2} \sin^2\left(\frac{\omega_j t}{2}\right) \coth\left(\frac{\beta\omega_j}{2}\right) \quad (3.41)$$

$$\frac{d\Gamma(t)}{dt} = \gamma(t) = \sum_j \frac{\lambda_j^2}{\omega_j} \sin(\omega_j t) \coth\left(\frac{\beta\omega_j}{2}\right) \quad (3.42)$$

we have

$$|v(t)|^2 = |v|^2 e^{-2\Gamma(t)} \quad (3.43)$$

$$\text{Re}(v'(t)v^*(t)) = \frac{1}{2} \partial_t |v(t)|^2 = -|v(t)|^2 \gamma(t). \quad (3.44)$$

We can then calculate  $\sigma(t, \rho, \nu)$  with formula (1.44)

$$\begin{aligned} \sigma(t, \rho, \nu) &= \frac{\alpha(t)\alpha'(t) + \text{Re}(v'(t)v^*(t))}{\sqrt{\alpha^2(t) + |v(t)|^2}} \\ &= \frac{-\gamma(t)|v(t)|^2 e^{-2\Gamma(t)}}{\sqrt{\alpha^2 + |v(t)|^2 e^{-2\Gamma(t)}}} \end{aligned} \quad (3.45)$$



We now need to maximize  $\sigma$ . It is clear again that  $v \neq 0$  and only for  $t \in (0, \infty)$  such that  $\gamma(t) < 0$  we have contributions to  $N(\Phi)$ . As in the previous case we have maximization for  $\alpha = 0$  and  $v = 1$ . Thus we get again

$$\begin{aligned}
N(\Phi) &= \max_{\rho(0), \nu(0)} \int_{\gamma(t) < 0} \sigma(t, \rho, \nu) dt \\
&= \max_{\alpha, v} \int_{\gamma(t) < 0} \frac{-\gamma(t)|v|^2 e^{-2\Gamma(t)}}{\sqrt{\alpha^2 + |v|^2 e^{-2\Gamma(t)}}} dt \\
&= \int_{\gamma(t) < 0} -\gamma(t) e^{-\Gamma(t)} dt \\
&= \sum_{k \geq 1} e^{-\Gamma(b_k)} - e^{-\Gamma(a_k)},
\end{aligned} \tag{3.46}$$

where again  $(a_k, b_k)$  are the intervals where  $\gamma(t) < 0$ . We will assume  $\omega_j = \omega$ ,  $\forall j$  to calculate the non-Markovianity  $N(\Phi)$  here. Defining

$$d = \frac{\coth(\frac{\beta\omega}{2}) \sum_j \lambda_j^2}{\omega} > 0, \quad \text{as } \omega > 0 \tag{3.47}$$

we can write

$$\gamma(t) = d \sin(\omega t) \quad \text{and} \tag{3.48}$$

$$\Gamma(t) = \frac{2d}{\omega} \sin^2\left(\frac{\omega t}{2}\right). \tag{3.49}$$

Finding now  $(a_k, b_k)$  such that  $\gamma(t) < 0$  we have (recall  $d > 0$  and  $\omega > 0$ )

$$\gamma(t) = d \sin(\omega t) < 0 \Leftrightarrow \sin(\omega t) < 0 \tag{3.50}$$

$$\Leftrightarrow t \in \left(\frac{(2k-1)\pi}{\omega}, \frac{2k\pi}{\omega}\right), k \in \mathbb{Z}. \tag{3.51}$$

Thus

$$(a_k, b_k) = \left(\frac{\pi}{\omega}(2k-1), \frac{2\pi}{\omega}k\right) \text{ for } k \in \mathbb{N}. \tag{3.52}$$

We now have the same situation as in section 3.1 and can calculate with initial states

$$\rho(0) = |\Theta\rangle \langle \Theta| = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \quad (3.53)$$

$$\nu(0) = |\chi\rangle \langle \chi| = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \quad (3.54)$$

and

$$\Gamma(b_k) = \Gamma\left(\frac{2k\pi}{\omega}\right) = 0 \quad (3.55)$$

$$\Gamma(a_k) = \Gamma\left(\frac{(2k-1)\pi}{\omega}\right) = \frac{2d}{\omega} \quad (3.56)$$

that

$$\begin{aligned} N(\Phi) &= \sum_{k \in \mathbb{N}} e^{-\Gamma(b_k)} - e^{-\Gamma(a_k)} \\ &= \sum_{k \in \mathbb{N}} \left(1 - e^{-\frac{2d}{\omega}}\right) \\ &= \infty, \text{ as } d > 0. \end{aligned} \quad (3.57)$$

Hence  $N(\Phi)$  diverges if we have a system of a spin coupled to a finite number of quantum harmonic oscillators with the same frequencies  $\omega$ .

From (3.47) it is clear that (3.57) reduces to (3.32) in the case of a single harmonic oscillator.

### 3.3 Spin coupled to bosonic field

The system of a spin coupled to a free bosonic field is governed by the Hamiltonian

$$H = \frac{\epsilon}{2} \sigma_z + H_E + \frac{\lambda}{2} \sigma_z \otimes \varphi(g), \quad (3.58)$$

where

$$H_E = \int_{\mathbb{R}^3} \omega(k) a^*(k) a(k) d^3k, \quad \varphi(g) = \int_{\mathbb{R}^3} (g(k) a^*(k) + \bar{g}(k) a(k)) d^3k. \quad (3.59)$$

Using formula (1.44) for

$$\sigma(t, \rho, \nu) = \frac{\alpha(t)\alpha'(t) + \operatorname{Re}(v'(t)v^*(t))}{\sqrt{\alpha^2(t) + |v(t)|^2}} \quad (3.60)$$

$$= \frac{-\gamma(t)|v|^2 e^{-2\Gamma(t)}}{\sqrt{\alpha^2 + |v|^2 e^{-2\Gamma(t)}}}. \quad (3.61)$$

and noting that  $N(\Phi)$  maximizes for  $\alpha = 0$  and  $|v| = 1$  (see page 43 f.) for two initial states  $\rho(0)$  and  $\nu(0)$  we arrive at

$$\begin{aligned} N(\Phi) &= \max_{\rho(0), \nu(0)} \int_{\gamma(t) < 0} \sigma(t, \rho, \nu) dt \\ &= \max_{\alpha, v} \int_{\gamma(t) < 0} \frac{-\gamma(t)|v|^2 e^{-2\Gamma(t)}}{\sqrt{\alpha^2 + |v|^2 e^{-2\Gamma(t)}}} \\ &= \int_{\gamma(t) < 0} -\gamma(t) e^{-\Gamma(t)} dt \\ &= \sum_{n \geq 1} e^{-\Gamma(b_n)} - e^{-\Gamma(a_n)}, \end{aligned} \quad (3.62)$$

with  $\Gamma(t)$  given by (2.118) and  $\gamma(t)$  by (2.119) respectively. Again  $(a_n, b_n)$  are the time intervals in which  $\gamma(t) < 0$ . Now the question is again *when is  $\gamma(t) < 0$ ?*

We need to specify the spectral density  $J(\omega)$  to be able to calculate  $N(\Phi)$ . Considering low temperature from here on ( $\beta\omega \rightarrow \infty$ ), we have  $\coth\left(\frac{\beta\omega}{2}\right) \approx 1$  and choose firstly as a spectral density

$$J(\omega) = \pi\omega^s \chi(\omega \leq \omega_0), \quad s > 0, \quad (3.63)$$

with  $\omega_0 > 0$  some cutoff frequency. As far as I know this case has not been discussed in the literature. With (2.118) and (2.119) we set for all  $s > 0$

$$\gamma_s(t) = \int_0^\infty \frac{\sin(\omega t)}{\omega} \omega^s \chi(\omega \leq \omega_0) d\omega \quad (3.64)$$

$$= \int_0^{\omega_0} \sin(\omega t) \omega^{s-1} d\omega \quad \text{and} \quad (3.65)$$

$$\Gamma_s(t) = \int_0^{\omega_0} (1 - \cos(\omega t)) \omega^{s-2} d\omega. \quad (3.66)$$

For example for  $s = 1$  we have

$$\gamma_1(t) = \frac{1}{t} (1 - \cos(\omega_0 t)) \quad (3.67)$$

and clearly  $\gamma_1(t) \geq 0, \forall t$  and as such  $N(\Phi) = 0$  and this process is Markovian.

For  $s = 3$  we have

$$\gamma_3(t) = \frac{1}{t^3} (2\omega_0 t \sin(\omega_0 t) - (\omega_0^2 t^2 - 2) \cos(\omega_0 t) - 2) \quad (3.68)$$

$$\Gamma_3(t) = \frac{1}{t^2} \left( \frac{1}{2} \omega_0^2 t^2 - \cos(\omega_0 t) - \omega_0 t \sin(\omega_0 t) + 1 \right). \quad (3.69)$$

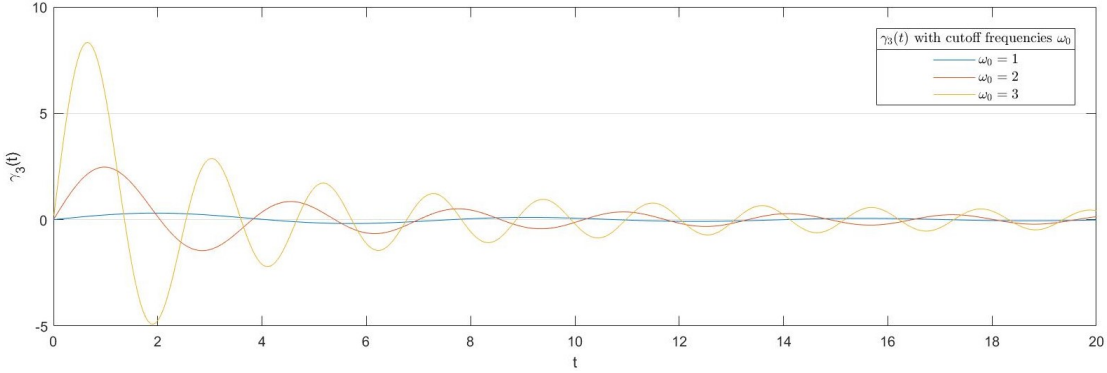


Figure 3.1: Graph of  $\gamma_3(t)$  with cutoff frequencies  $\omega_0 = 1, 2, 3$

One can see in fig. 3.1 that for various cutoff frequencies  $\omega_0$  we indeed have times such that  $\gamma_3(t) < 0$ . Analytically this isn't solvable. Note that since

$$N(\Phi) = \sum_{n \in \mathbb{N}} D(t_n^{\min}, \rho, \nu) - D(t_n^{\max}, \rho, \nu) \quad (3.70)$$

with  $\sigma(t, \rho, \nu) > 0$  for  $t \in (t_n^{\max}, t_n^{\min})$  it is sufficient to know the behavior of the trace distance  $D$  for large  $t$ , if we want to check that  $N(\phi) = \infty$ .

We will focus on the case with  $\omega_0 = 5$ . In Figure 3.2 we see plotted  $\gamma_3(t)$  and  $\Gamma_3(t)$  with  $\omega_0 = 5$ . Define  $\gamma_s^{\omega_0}$  as the function where  $s$  and  $\omega_0$  are fixed and similarly  $\Gamma_s^{\omega_0}$ . By  $x_n$  we denote the roots of  $\gamma_3^5(t)$ .

For large  $t$  we see from (3.68) that  $\gamma_3^5(t)$  behaves like  $\overline{\gamma_3^5} := -\frac{25}{t} \cos(5t)$  (by the overline symbol  $\overline{\phantom{x}}$  we describe the behavior of the function for large  $t$ ) and consequently  $\Gamma_3^5(t)$  behaves like

$$\overline{\Gamma_3^5} := \frac{25}{2} - \frac{5}{t} \sin(5t). \quad (3.71)$$

Plotting  $\overline{\Gamma_3^5}$  with  $\Gamma_3^5$  (see fig. 3.3) and  $\overline{\gamma_3^5}$  with  $\gamma_3^5$  (see fig. 3.4) we see that they coincide very well for large  $t$ .

We can thus approximate for large  $t$  the  $n$ -th root  $x_n$  of  $\gamma_3^5$  by that of  $\overline{\gamma_3^5}$ ,

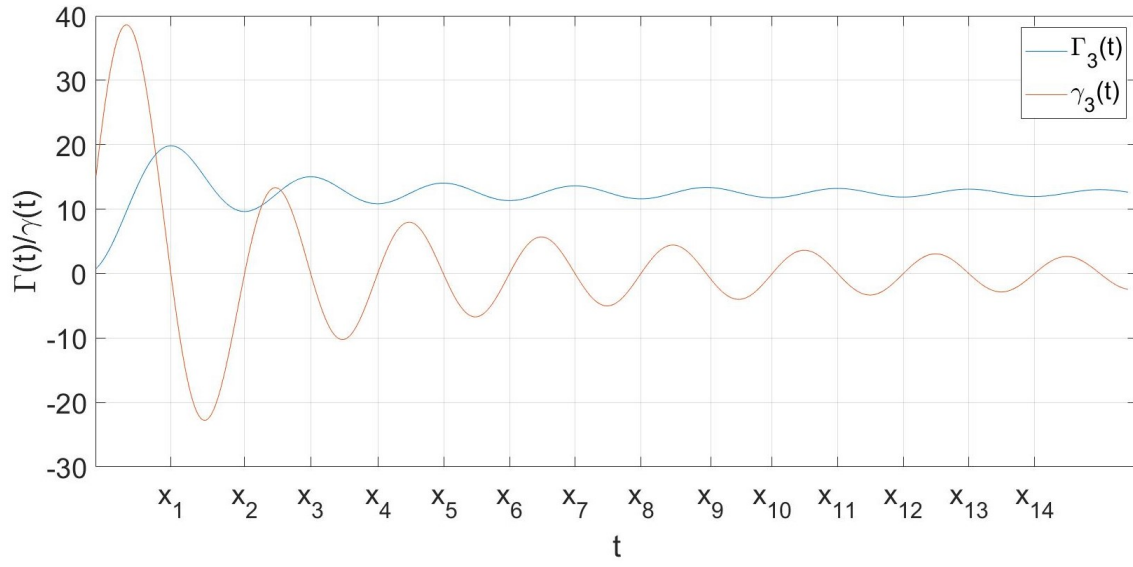


Figure 3.2:  $\Gamma_3(t)$  and  $\gamma_3(t)$  with  $\omega_0 = 5$

$$x_n = \frac{(n + \frac{1}{2})\pi}{5}, \quad n \in \mathbb{N} \quad (3.72)$$

and

$$\gamma_3^5(t) < 0 \Leftrightarrow t \in (x_{2n-1}, x_{2n}). \quad (3.73)$$

Calculating  $N(\Phi)$  using (3.62) with

$$\Gamma(b_n) \approx \overline{\Gamma}_3^5(x_{2n}) = +\frac{25}{(2n - \frac{1}{2})\pi} + \frac{25}{2} \quad (3.74)$$

$$\Gamma(a_n) \approx \overline{\Gamma}_3^5(x_{2n-1}) = -\frac{25}{(2n + \frac{1}{2})\pi} + \frac{25}{2} \quad (3.75)$$

and the fact that for large  $t$  we have

$$\Gamma_3^5(t) \approx \overline{\Gamma}_3^5(t). \quad (3.76)$$

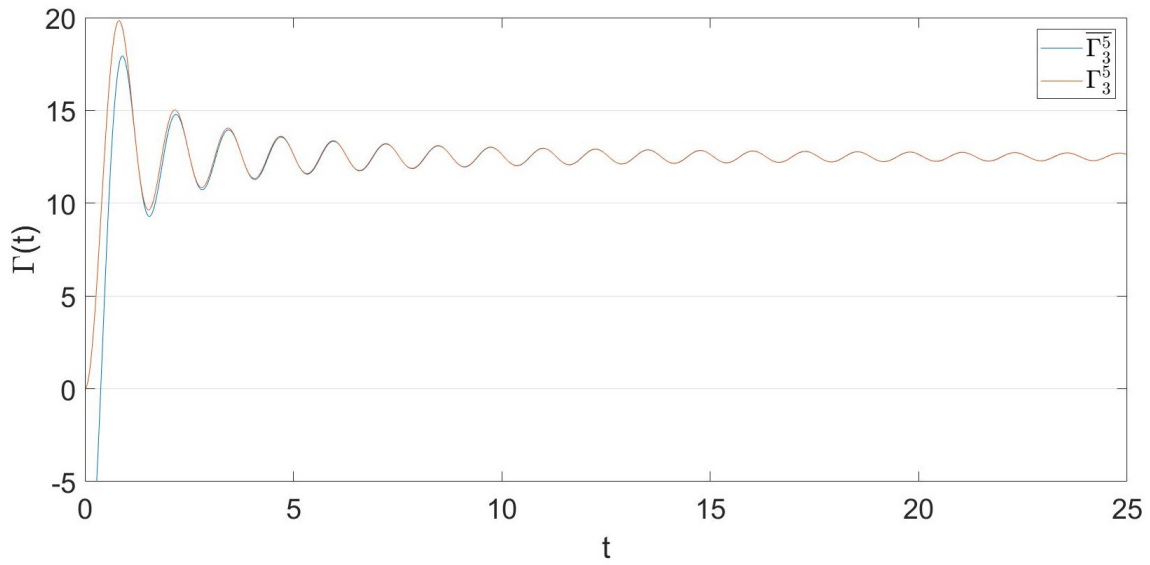


Figure 3.3: Comparison for large  $t$

$\Gamma_3^5(t)$  and  $\overline{\Gamma}_3^5(t)$  in comparison

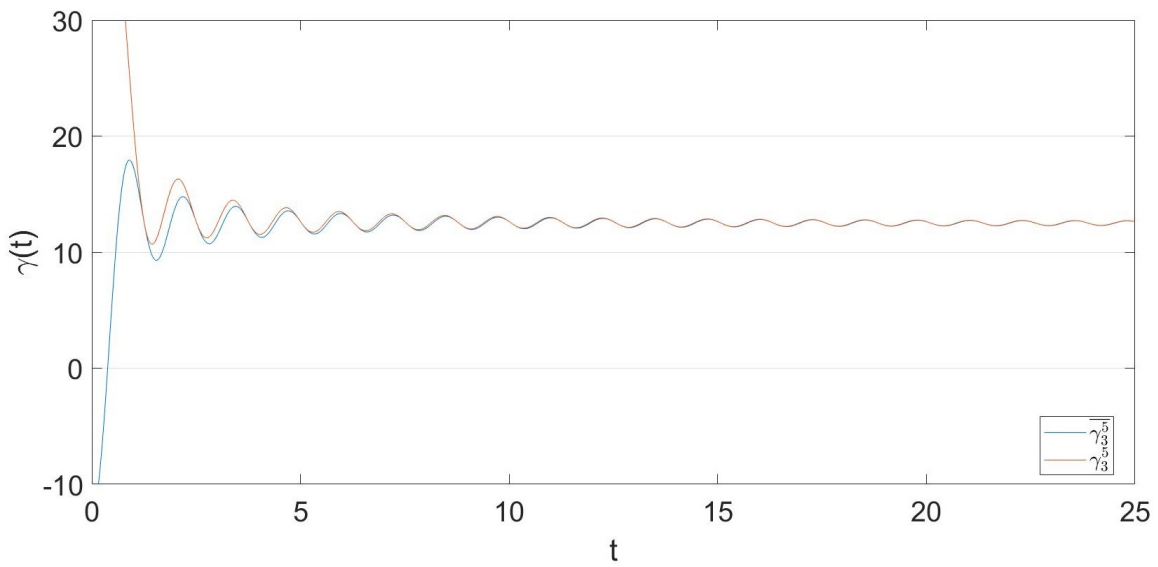


Figure 3.4: Comparison for large  $t$

$\gamma_3^5(t)$  and  $\overline{\gamma}_3^5(t)$  in comparison

Using additionally  $e^x \approx 1 + x$  for  $x \ll 1$  we can approximate

$$\begin{aligned}
N(\Phi) &= \sum_{n \geq 1} e^{-\Gamma_3^5(x_{2n})} - e^{-\Gamma_3^5(x_{2n-1})} \\
&\approx \sum_{n \geq 1} e^{-\overline{\Gamma}_3^5(x_{2n})} - e^{-\overline{\Gamma}_3^5(x_{2n-1})} \\
&= e^{-\frac{25}{2}} \sum_{n \geq 1} e^{+\frac{25}{(2n+\frac{1}{2})\pi}} - e^{-\frac{25}{(2n-\frac{1}{2})\pi}} \\
&\approx e^{-\frac{25}{2}} \sum_{n \geq 1} \frac{25}{(2n+\frac{1}{2})\pi} + \frac{25}{(2n-\frac{1}{2})\pi} + \mathcal{O}\left(\frac{1}{n^2}\right) \\
&= e^{-\frac{25}{2}} \sum_{n \geq 1} \frac{100n}{4\pi n^2 - \frac{1}{4}\pi} + \mathcal{O}\left(\frac{1}{n^2}\right) \\
&\approx e^{-\frac{25}{2}} \sum_{n \geq 1} \frac{25}{n\pi} + \mathcal{O}\left(\frac{1}{n^2}\right) \\
&= +\infty.
\end{aligned} \tag{3.77}$$

We see that the series  $\sum_{n \geq 1} e^{-\Gamma_3^5(x_{2n})} - e^{-\Gamma_3^5(x_{2n-1})}$  diverges and we have infinite non-Markovianity  $N(\Phi)$ . This means that for the spectral density  $J(\omega) = \omega^3 \chi_{\omega \leq 5}$  we can never approximate the master equation through a Markovian one.

References [14, 13, 1] have discussed the case when we choose a spectral density of the form

$$J(\omega) = \frac{\omega^s}{\omega_0^{s-1}} e^{-\omega/\omega_0}, \tag{3.78}$$

where  $s > 0$ . I will briefly summarize the results for this case, as we have a finite non-Markovianity  $N(\Phi)$  here.

We have

$$\Gamma_s(t) = \int_0^\infty (1 - \cos(\omega t)) \frac{\omega^{s-2}}{\omega_0^{s-1}} e^{-\frac{\omega}{\omega_0}} d\omega \tag{3.79}$$

$$\gamma_s(t) = \int_0^\infty \sin(\omega t) \frac{\omega^{s-1}}{\omega_0^{s-1}} e^{-\frac{\omega}{\omega_0}} d\omega. \tag{3.80}$$

Using the formulas from section C we get

$$\Gamma_s(t) = \tilde{\Gamma}(s-1) \left( 1 - \frac{\cos((s-1) \arctan(t\omega_0))}{(t^2\omega_0^2 + 1)^{\frac{s-1}{2}}} \right) \quad (3.81)$$

$$\gamma_s(t) = \frac{\omega_0 \tilde{\Gamma}(s)}{(t^2\omega_0^2 + 1)^{\frac{s}{2}}} \sin(s \arctan(t\omega_0)), \quad (3.82)$$

where  $\tilde{\Gamma}(s)$  is the Euler gamma function  $\int_0^\infty e^{-t} t^{s-1} dt$ . Since  $\arctan(\omega_0 t) \in (0, \frac{\pi}{2})$ , as it is the principal branch only, for  $t > 0$  we have that

$$\sin(s \arctan(\omega_0 t)) \in (0, 1) \text{ for } s \leq 2. \quad (3.83)$$

Hence  $\gamma_s(t) > 0$  for  $s \leq 2$  and the process is Markovian in the sub-ohmic  $0 < s < 1$  and ohmic  $s = 1$  case. Only for  $s > 2$ , the super-ohmic case, do we have a non-Markovian process. We denote the critical parameter for which the switch from Markovian to non-Markovian behavior occurs as  $s_{crit}$ . In this model we have assumed low temperature,  $\frac{1}{T} \approx \beta\omega \rightarrow \infty$  and concluded  $s_{crit} = 2$ . This value actually depends on the temperature  $T$ . In [14] it has been shown numerically that for an increase of temperature we also encounter an increase of  $s_{crit}$  until we reach its maximum value of  $s_{crit} = 3$  for an infinite temperature.

We will first show that the number of roots of  $\gamma_s(t)$  depends on the parameter  $s$  for this spectral density. Let  $y(t) := \arctan(\omega_0 t) \in (0, \frac{\pi}{2})$  for  $t > 0$  and consider

$$w(y) := \sin(sy). \quad (3.84)$$

Then for  $s > 2$

$$sy \in (0, \frac{s\pi}{2}) \quad (3.85)$$

and  $w(y)$  has  $\lceil \frac{s}{2} \rceil$  many roots at  $n\pi$  for  $n < \lceil \frac{s}{2} \rceil$  and  $n \in \mathbb{N}$ . We thus have possible intervals such that  $\gamma_s(t) < 0$  for  $s > 2$ . Then for  $\gamma_s(t)$  we get

$$\gamma_s(t) = 0 \Leftrightarrow sy(t) = n\pi \quad (3.86)$$

$$\Leftrightarrow \arctan(\omega_0 t) = \frac{n\pi}{s} \quad (3.87)$$

$$\Leftrightarrow t = \frac{\tan\left(\frac{n\pi}{s}\right)}{\omega_0} \text{ for } n \in \mathbb{N}, n < \lceil \frac{s}{2} \rceil. \quad (3.88)$$



For example for  $s = 3$  and  $s = 4$  we have one zero at  $t = \frac{\sqrt{3}}{\omega_0}$  and  $t = \frac{1}{\omega_0}$  respectively. More generally it has been shown in [1] that the intervals such that  $\gamma_s(t) < 0$  for  $t \in (a_1, b_1)$  are given by

$$2 < s \leq 4 : a_1 = \frac{\tan\left(\frac{\pi}{s}\right)}{\omega_0} \quad b_1 = \infty \quad (3.89)$$

$$4 < s \leq 6 : a_1 = \frac{\tan\left(\frac{\pi}{s}\right)}{\omega_0} \quad b_1 = \frac{\tan\left(\frac{2\pi}{s}\right)}{\omega_0} \quad (3.90)$$

For  $s > 6$  we have more than one interval in which  $\gamma_s(t) < 0$ .

The analytic expressions for  $\Gamma(t)$  at the interval boundaries are

$$\Gamma(a_1) = \tilde{\Gamma}(s-1) \left(1 + \cos^s\left(\frac{\pi}{s}\right)\right) \quad (3.91)$$

$$2 < s \leq 4 : \Gamma(b_1) = \tilde{\Gamma}(s-1) \quad (3.92)$$

$$4 < s \leq 6 : \Gamma(b_1) = \tilde{\Gamma}(s-1) \left(1 - \cos^s\left(\frac{2\pi}{s}\right)\right). \quad (3.93)$$

We will study the case  $s = 3$  more explicitly now. We have

$$\gamma_3(t) = \frac{2\omega_0}{(t^2\omega^2 + 1)^{\frac{3}{2}}} \sin(3 \arctan(t\omega_0)) \quad (3.94)$$

$$\Gamma_3(t) = 1 - \frac{\cos(2 \arctan(t\omega_0))}{(t^2\omega_0^2 + 1)}. \quad (3.95)$$

Now using (3.62) to calculate the non-Markovianity  $N(\Phi)$ , the roots in equation (3.89) and the analytic expressions (3.91) and (3.92), we calculate

$$\begin{aligned} N(\Phi) &= \int_{\gamma^3(t) < 0} \sigma(t, \rho, \nu) dt \\ &= \int_{\frac{\tan(\frac{\pi}{3})}{\omega_0}}^{\infty} -\gamma^3(t) e^{-\Gamma^3(t)} dt \\ &= e^{-\tilde{\Gamma}(2)} - e^{-\tilde{\Gamma}(2)(1+\cos^3(\frac{\pi}{3}))} \\ &= 0.0432. \end{aligned} \quad (3.96)$$

In Fig. 3.5 we see plotted the calculated Non-Markovianity  $N(\Phi)$  for different choices of  $s$ . It is interesting to note that for  $s \approx 3.7$  we reach the maximum for  $N(\Phi)$  and for  $s \approx 6$  we have  $N(\Phi) \approx 0$ .

We see here that we can have a finite measure  $N(\Phi)$  and memory effects are present in this case.

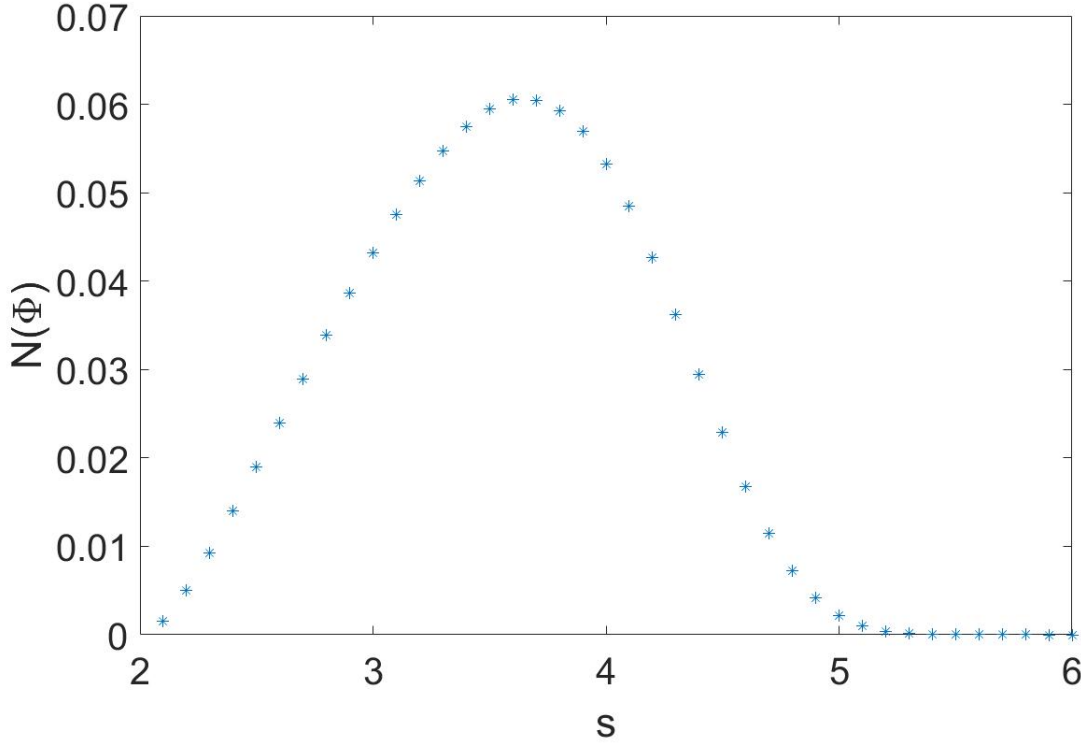


Figure 3.5:  $N(\Phi)$  in dependence of  $s$

## Summary

In this chapter we have calculated the non-Markovianity  $N$  for the three cases of chapter 2. A spin coupled to finite many oscillators always gives an infinite non-Markovianity  $N$ . In the case of the spin coupled to a free bosonic field though the result for  $N$  is not unique. We need to distinguish between different spectral density functions  $J(\omega)$ . For a spectral density of form (3.63) for  $s = 3$  and  $\omega_0 = 5$  we calculated an infinite non-Markovianity  $N$  (see (3.77)). Choosing a spectral density of the form (3.78) we obtain finite non-Markovianity for different choices of  $s$ . In summary we see that for different choices of the spectral density  $J(\omega)$  we obtain a range between 0 and  $\infty$  for the non-Markovianity,  $N$ . For comparison I will also reference [5] which discusses the case of a Lorentzian spectral density

$$J(\omega) = \frac{\gamma_0 \lambda^2}{2\pi ((\omega_0 - \Delta - \omega)^2 + \lambda^2)} \quad (3.97)$$

with  $\Delta$  being the detuning amount of the center,  $\omega_0$  the transition frequency and works in the weak coupling limit  $\gamma_0/\lambda = 0.01$  (damped Jaynes-Cummings model). In this case

results are obtained through numerical methods and the findings for the non-Markvoianity depending on the variable  $\Delta/\lambda$  are within a finite range, i.e.  $0 \leq N < \infty$ .

# Chapter 4

## Mean field evolution of open quantum system

As mentioned in the introduction we are interested in systems that can be described through open quantum systems which don't assume a Markovian approximation, hence are non-Markovian. So far we have dealt with only a single spin coupled to different environments. Systems of interest though in physics, biology and chemistry are often very complex and involve a large number of quantum particles coupled to an environment and a large number of degrees of freedom. The master equation for such a system is extremely difficult to solve and one can try to approximate the equation in various ways. One such approach is the *mean field approximation*. In this approximation we sacrifice the 'easy' evolution of the single particle for a more complicated one, but trade the complexity of the system (large number of particles) for particle independence. This is achieved by approximating the effect all other particles have on one individual particle by just a single averaged effect.

### 4.1 Description of the problem

We want to measure the non-Markovianity  $N(\Phi)$  for a system of  $N_{\text{tot}}$  identical quantum particles coupled to local and common reservoirs in thermal equilibrium. In the work by Berman and Merkli in [24] the dynamics in the mean field evolution of such a system is explicitly solved. The following situation is considered.

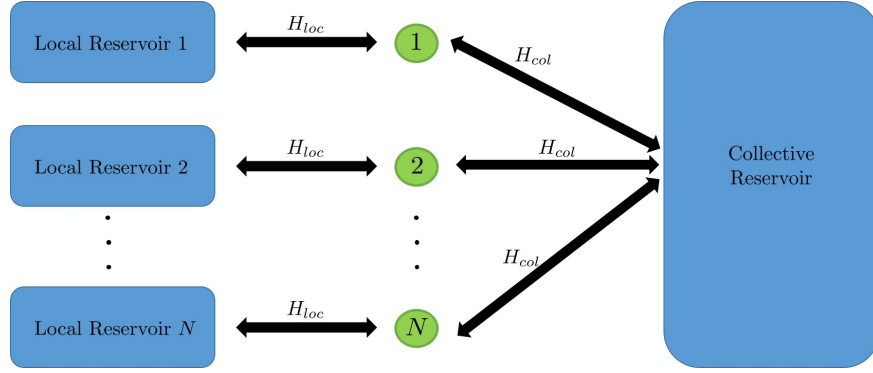


Figure 4.1: Mean Field Case

$N_{\text{tot}}$  particles, each coupled to a local reservoir through Hamiltonian  $H_{loc}$  and also individually coupled to the common reservoir through the Hamiltonian  $H_{col}$ . No direct coupling between particles.

The Hilbert Space of the total system is

$$\mathbb{C}^2 \otimes \dots \otimes \mathbb{C}^2 \otimes \mathcal{F} \otimes \mathcal{F} \otimes \dots \otimes \mathcal{F}, \quad (4.1)$$

where  $\mathbb{C}^2$  is the Hilbert space of the single particle ( $N_{\text{tot}}$  times) and  $\mathcal{F}$  is the Hilbert space of the reservoir ( $N_{\text{tot}}$  local and one common reservoir). The dynamics is governed by the mean field scaled Hamiltonian

$$H_N = \sum_{j=1}^{N_{\text{tot}}} A_j + \sum_{j=1}^{N_{\text{tot}}} K_j + K \quad (4.2)$$

$$+ \sum_{j=1}^{N_{\text{tot}}} \chi_j V_j \otimes \varphi_j(f_j) \quad (4.3)$$

$$+ \frac{\chi_c}{\sqrt{N_{\text{tot}}}} \sum_{j=1}^{N_{\text{tot}}} W_j \otimes \varphi(f). \quad (4.4)$$

The first term (4.2) describes the free evolution of the single particle (Hamiltonian  $A_j$ ), free evolution of the local ( $K_j$ ) and collective ( $K$ ) reservoir, (4.3) is the sum of Hamiltonians of each single particle  $j$  interacting with its local reservoir and (4.4) describes the interaction between each particle  $j$  and the collective reservoir. We see here that the collective coupling (4.4) is scaled in the mean field way by the factor  $\frac{\chi_c}{\sqrt{N_{\text{tot}}}}$ .

We now consider the specific case with  $N_{\text{tot}}$  spins and the common and all local reservoirs given by a heat bath, modeled through a spatially infinitely free Bose gas

initially in thermal equilibrium all at the same temperature  $T = 1/\beta$ . For a more detailed description of the free field evolution and single spin evolution see section 2.3, we just remind here that for all  $j$

$$A_j = \frac{\omega}{2} \sigma_z \quad (4.5)$$

$$K_j = K = \int_{\mathbb{R}^3} |k| a^*(k) a(k) d^3k, \quad (4.6)$$

with  $\omega > 0$  being the frequency of a spin. The interaction terms (4.3) and (4.4) are the same for each spin and are specified with  $\varphi(f)$  being the field operator from section 2.3 for some form factor  $f \in L^2(\mathbb{R}^3, d^3k)$  and

$$V_j = W_j = \frac{1}{2} \sigma_z, \quad \forall j. \quad (4.7)$$

We take all coupling constants  $\chi_j$  to the local reservoirs to be equal  $\chi_j = \chi_l$ , as well as the coupling constant  $\chi_c$  to the collective reservoir to be any real number, not necessarily small.

The main result of [24] is the following: Consider now a fixed  $n$ -particle sub-system of the large  $N_{\text{tot}}$ -particle system starting in a product initial state

$$\rho_0 \otimes \cdots \otimes \rho_0 \quad (N_{\text{tot}}\text{-fold}). \quad (4.8)$$

The reduced  $n$ -particle state evolves according to

$$\rho_{n, N_{\text{tot}}}(t) = \text{Tr}_{n+1, N_{\text{tot}}} \left( e^{-itH_{N_{\text{tot}}}} \rho_0 \otimes \cdots \otimes \rho_0 \otimes \rho_{\vec{R}} e^{itH_{N_{\text{tot}}}} \right), \quad (4.9)$$

where  $\rho_{\vec{R}}$  is the product state of the common reservoir and all  $N_{\text{tot}}$  local reservoirs. Here we take the trace,  $\text{Tr}_{n+1, N_{\text{tot}}}$ , over all other particles  $n+1, n+2, \dots, N_{\text{tot}}$  and all reservoirs. We now keep  $n$  fixed and let  $N_{\text{tot}} \rightarrow \infty$ . The result is that the reduced  $n$ -particle state at any time  $t$  is a factorized one-particle state. We denote this by

$$\rho_{n, N_{\text{tot}}}(t) \rightarrow \rho_t \otimes \cdots \otimes \rho_t, \quad N_{\text{tot}} \rightarrow \infty, \quad (n\text{-fold}). \quad (4.10)$$

Each single spin density matrix  $\rho_t$ , qubits in our case, evolves according to the Hartree-Lindblad equation (Theorem 1.1 in [24])

$$i\dot{\rho}_t = \frac{\omega}{2}[\sigma_z, \rho_t] + \frac{1}{2}\chi_c^2\dot{S}(t) \text{Tr}_2[\sigma_z \otimes \sigma_z, \rho_t \otimes \rho_t] - \frac{i}{4}\chi_l^2\dot{\Gamma}_l(t)[\sigma_z, [\sigma_z, \rho_t]]. \quad (4.11)$$

The first term on the right side derives from the free evolution of the spin  $j$ , the second term is the mean field averaged effect through the effective operator  $W_{\text{eff}} = \frac{1}{4}\dot{S}(t)\sigma_z \otimes \sigma_z$  on the individual particle  $j$  from all other particles through the collective reservoir and the third term originates from the coupling to the local reservoir. The quantities  $S(t)$  and  $\Gamma_l(t)$  are given by

$$\Gamma_l(t) = \int_{\mathbb{R}^3} |f(k)|^2 \coth(\beta|k|/2) \frac{\sin^2(|k|t/2)}{|k|^2} d^3k \quad (4.12)$$

$$S(t) = \frac{1}{2} \int_{\mathbb{R}^3} |f(k)|^2 \frac{|k|t - \sin(|k|t)}{|k|^2} d^3k. \quad (4.13)$$

Considering the initial state  $\rho(0) = \begin{pmatrix} p & \rho_{12}(0) \\ \rho_{12}^*(0) & 1-p \end{pmatrix}$  the solution to (4.11) for a single spin density matrix is given by

$$\rho(t) = \begin{pmatrix} p & \rho_{12}(0)c_{12}(t) \\ \rho_{12}^*(0)c_{12}^*(t) & 1-p \end{pmatrix} \quad (4.14)$$

with

$$c_{12}(t) = e^{-i\omega t} e^{-\frac{i}{2}\chi_c^2(2p-1)S(t)} e^{-\chi_l^2\Gamma_l(t)}. \quad (4.15)$$

## 4.2 Trace distance and asymptotic behavior

Here we will calculate the quantities  $D(t, \rho, \nu)$  and  $\sigma(t, \rho, \nu)$  to use in the following section for the non-Markovianity  $N(\Phi)$ . We will also calculate the asymptotic behavior for large  $t$  of these quantities to use for calculations for the quantum system described in section 4.1. Let

$$\rho(t) = \begin{pmatrix} p & \rho_{12}(0)c_{12}^p(t) \\ \rho_{12}^*(0)(c_{12}^p(t))^* & 1-p \end{pmatrix} \quad (4.16)$$

and

$$\nu(t) = \begin{pmatrix} q & \nu_{12}(0)c_{12}^q(t) \\ \nu_{12}^*(0)(c_{12}^q(t))^* & 1-q \end{pmatrix} \quad (4.17)$$

be the density matrices at time  $t$ , with  $c_{12}^{p,q}(t)$  as in (4.15), with initial states

$$\rho(0) = \begin{pmatrix} p & \rho_{12}(0) \\ \rho_{12}^*(0) & 1-p \end{pmatrix} \quad (4.18)$$

and

$$\nu(0) = \begin{pmatrix} q & \nu_{12}(0) \\ \nu_{12}^*(0) & 1-q \end{pmatrix}. \quad (4.19)$$

For the calculation of  $\sigma(t, \rho, \nu)$  we need

$$\frac{d}{dt}\Gamma_l(t) := \gamma(t) = \frac{1}{2} \int_{\mathbb{R}^3} |f(k)|^2 \coth(\beta|k|/2) \frac{\sin(|k|t)}{|k|} d^3k \quad (4.20)$$

$$\frac{d}{dt}S(t) := s(t) = \frac{1}{2} \int_{\mathbb{R}^3} |f(k)|^2 \frac{1 - \cos(|k|t)}{|k|} d^3k. \quad (4.21)$$

We have (compare to (1.34), (1.35))

$$\alpha(t) = \rho_{11} - \nu_{11} = p - q \quad (4.22)$$

$$v(t) = \rho_{12}(0)c_{12}^p(t) - \nu_{12}(0)c_{12}^q(t) \quad (4.23)$$

$$= e^{-i\omega t} e^{-\chi_l^2 \Gamma_l(t)} \left( \rho_{12}(0) e^{-\frac{i}{2} \chi_c^2 S(t)(2p-1)} - \nu_{12}(0) e^{-\frac{i}{2} \chi_c^2 S(t)(2q-1)} \right) \quad (4.24)$$

and using lemma 1.2.3 gives us the trace distance as

$$D(t, \rho, \nu) = \sqrt{\alpha(t)^2 + |v(t)|^2}. \quad (4.25)$$

The rate of change  $\sigma(t, \rho, \nu)$  is given by equation (1.44)

$$\sigma(t, \rho, \nu) = \frac{\alpha(t)\alpha'(t) + \frac{1}{2}(|v(t)|^2)'}{\sqrt{\alpha^2(t) + |v(t)|^2}} =: \frac{Z(t)}{W(t)}. \quad (4.26)$$

Calculating the necessary quantities for  $\sigma$  and writing for short  $\rho_{12} \equiv \rho_{12}(0)$  and similarly for  $\nu_{12}(0)$  results in:



$$|v(t)|^2 = e^{-2\chi_l^2 \Gamma_l(t)} \left[ |\rho_{12}|^2 + |\nu_{12}|^2 - 2\text{Re} \left( \rho_{12}^* \nu_{12} e^{i\chi_c^2 S(t)(p-q)} \right) \right] \quad (4.27)$$

$$= e^{-2\chi_l^2 \Gamma_l(t)} \left[ |\rho_{12}|^2 + |\nu_{12}|^2 - 2\text{Re}(\rho_{12}^* \nu_{12}) \cos(\chi_c^2 S(t)(p-q)) \right. \\ \left. + 2\text{Im}(\rho_{12}^* \nu_{12}) \sin(\chi_c^2 S(t)(p-q)) \right] \quad (4.28)$$

$$(|v(t)|^2)' = -2\chi_l^2 \gamma(t) |v(t)|^2 + 2e^{-2\chi_l^2 \Gamma_l(t)} \chi_c^2 s(t)(p-q) \times \\ \{ \text{Re}(\rho_{12}^* \nu_{12}) \sin(\chi_c^2 S(t)(p-q)) + \text{Im}(\rho_{12}^* \nu_{12}) \cos(\chi_c^2 S(t)(p-q)) \} \quad (4.29)$$

and we can write

$$Z(t) = -\chi_l^2 \gamma(t) |v(t)|^2 + e^{-2\chi_l^2 \Gamma_l(t)} \chi_c^2 s(t)(p-q) \times \\ \{ \text{Re}(\rho_{12}^* \nu_{12}) \sin(\chi_c^2 S(t)(p-q)) + \text{Im}(\rho_{12}^* \nu_{12}) \cos(\chi_c^2 S(t)(p-q)) \} \quad (4.30)$$

$$W(t) = \sqrt{(p-q)^2 + e^{-2\chi_l^2 \Gamma_l(t)} [|\rho_{12}|^2 + |\nu_{12}|^2 - 2\text{Re}(\rho_{12}^* \nu_{12} e^{i\chi_c^2 S(t)(p-q)})]}. \quad (4.31)$$

As shown in appendix B we can rewrite

$$\Gamma_l(t) = \frac{1}{\pi} \int_0^\infty J(\omega) \frac{1 - \cos(\omega t)}{\omega^2} \coth\left(\frac{\beta\omega}{2}\right) d\omega \quad (4.32)$$

$$\gamma(t) = \frac{1}{\pi} \int_0^\infty J(\omega) \frac{\sin(\omega t)}{\omega} \coth\left(\frac{\beta\omega}{2}\right) d\omega \quad (4.33)$$

$$S(t) = \frac{1}{\pi} \int_0^\infty J(\omega) \frac{\omega t - \sin(\omega t)}{\omega^2} d\omega \quad (4.34)$$

$$s(t) = \frac{1}{\pi} \int_0^\infty J(\omega) \frac{1 - \cos(\omega t)}{\omega} d\omega \quad (4.35)$$

with spectral density  $J(\omega)$ . To explicitly calculate  $N(\Phi)$  we need to specify the spectral density  $J(\omega)$  in the quantities  $\Gamma_l(t)$  and  $S(t)$ . We will use a ohmic-like spectral density, with some reservoir cutoff frequency  $\omega_0 > 0$

$$J(\omega) = \frac{\omega^s}{\omega_0^{s-1}} e^{-\frac{\omega}{\omega_0}} \quad , s > 1. \quad (4.36)$$

We will only consider the super-ohmic case  $s > 1$  here. Considering low temperature ( $\beta\omega_0 \rightarrow \infty$ ), we have  $\coth\left(\frac{\beta\omega}{2}\right) \approx 1$  in the integrals (4.32)-(4.35) and thus

$$\Gamma_l(t) = \frac{1}{\pi} \int_0^\infty (1 - \cos(\omega t)) \frac{\omega^{s-2}}{\omega_0^{s-1}} e^{-\frac{\omega}{\omega_0}} d\omega \quad (4.37)$$

$$\gamma(t) = \frac{1}{\pi} \int_0^\infty \sin(\omega t) \frac{\omega^{s-1}}{\omega_0^{s-1}} e^{-\frac{\omega}{\omega_0}} d\omega \quad (4.38)$$

$$S(t) = \frac{1}{\pi} \int_0^\infty (\omega t - \sin(\omega t)) \frac{\omega^{s-2}}{\omega_0^{s-1}} e^{-\frac{\omega}{\omega_0}} d\omega \quad (4.39)$$

$$s(t) = \frac{1}{\pi} \int_0^\infty (1 - \cos(\omega t)) \frac{\omega^{s-1}}{\omega_0^{s-1}} e^{-\frac{\omega}{\omega_0}} d\omega. \quad (4.40)$$

Using the formulas from appendix C we have

$$\Gamma_l(t) = \frac{\tilde{\Gamma}(s-1)}{\pi} \left( 1 - \frac{\cos((s-1) \arctan(t\omega_0))}{(t^2\omega_0^2 + 1)^{\frac{s-1}{2}}} \right) \quad (4.41)$$

$$\gamma(t) = \frac{\omega_0 \tilde{\Gamma}(s)}{\pi(t^2\omega_0^2 + 1)^{\frac{s}{2}}} \sin(s \arctan(t\omega_0)) \quad (4.42)$$

$$S(t) = \frac{\tilde{\Gamma}(s-1)}{\pi} \left( \omega_0(s-1)t - \frac{\sin((s-1) \arctan(t\omega_0))}{(t^2\omega_0^2 + 1)^{\frac{s-1}{2}}} \right) \quad (4.43)$$

$$s(t) = \frac{\omega_0 \tilde{\Gamma}(s)}{\pi} \left( 1 - \frac{\cos(s \arctan(t\omega_0))}{(t^2\omega_0^2 + 1)^{\frac{s}{2}}} \right), \quad (4.44)$$

where  $\tilde{\Gamma}(s)$  is the Euler gamma function

$$\tilde{\Gamma}(s) = \int_0^\infty e^{-t} t^{s-1} dt. \quad (4.45)$$

The question now is again, *when is  $\sigma > 0$ ?* Since an analytic solution cannot be elaborated we will approximate the solution for large  $t$ . Remember that the non-Markovianity  $N(\Phi)$  is a series and for divergence of such we only need to know the behavior of the summands for large times and we can use approximations to calculate  $N(\Phi)$ . First recall the following Lemma

**Lemma 4.2.1.** *The product of a null sequence and a bounded sequence is a null sequence.*

With

$$\lim_{t \rightarrow \infty} \sin(s \arctan(t\omega_0)) = \sin\left(s \frac{\pi}{2}\right) \quad (4.46)$$

$$\lim_{t \rightarrow \infty} \frac{\omega_0 \tilde{\Gamma}(s)}{\pi(t^2\omega_0^2 + 1)^{\frac{s}{2}}} = 0 \quad (4.47)$$

for fixed  $\omega_0$  and fixed  $s > 1$  we have

$$\lim_{t \rightarrow \infty} \gamma(t) = 0. \quad (4.48)$$

We can then approximate for sufficiently large  $t$

$$\frac{\cos(s \arctan(t\omega_0))}{(t^2\omega_0^2 + 1)^{\frac{s}{2}}} \approx 0 \quad \text{and} \quad (4.49)$$

$$\frac{\sin((s-1) \arctan(t\omega_0))}{(t^2\omega_0^2 + 1)^{\frac{s-1}{2}}} \approx 0. \quad (4.50)$$

Taking this into consideration we can conclude that for large  $t$  the functions (4.41)-(4.44) behave like (by the overline symbol  $\overline{\phantom{x}}$  we describe the behavior of the function for sufficiently large  $t$ )

$$\overline{S}(t) = \frac{\tilde{\Gamma}(s)\omega_0}{\pi} t \quad (4.51)$$

$$\overline{\Gamma}_l = \frac{\tilde{\Gamma}(s-1)}{\pi} \quad (4.52)$$

$$\overline{s} = \frac{\tilde{\Gamma}(s)\omega_0}{\pi} \quad (4.53)$$

$$\overline{\gamma}(t) = 0. \quad (4.54)$$

Note here that the functions  $\overline{\Gamma}_l$  and  $\overline{s}$  do not depend on  $t$  and that  $\overline{s}$  is not the parameter

$s$  but the function  $s(t)$  for large  $t$ . Or using the asymptotic notation we write

$$S(t) = \frac{\tilde{\Gamma}(s)\omega_0}{\pi}t + O(t^{1-s}) \quad (4.55)$$

$$\Gamma_l(t) = \frac{\tilde{\Gamma}(s-1)}{\pi} + O(t^{1-s}) \quad (4.56)$$

$$s(t) = \frac{\tilde{\Gamma}(s)\omega_0}{\pi} + O(t^{-s}) \quad (4.57)$$

$$\gamma(t) = O(t^{-s}). \quad (4.58)$$

Taking this into consideration we can write for large  $t$

$$\begin{aligned} \overline{Z}(t) &= e^{-2\chi_l^2\tilde{\Gamma}_l}\chi_c^2\overline{s}(p-q) \times \left\{ Re(\rho_{12}^*\nu_{12}) \sin(\chi_c^2\overline{S}(t)(p-q)) \right. \\ &\quad \left. + Im(\rho_{12}^*\nu_{12}) \cos(\chi_c^2\overline{S}(t)(p-q)) \right\} \\ &= e^{-2\chi_l^2\frac{\tilde{\Gamma}(s-1)}{\pi}}\chi_c^2\frac{\tilde{\Gamma}(s)\omega_0}{\pi}(p-q) \times \left\{ Re(\rho_{12}^*\nu_{12}) \sin\left(\chi_c^2\frac{\tilde{\Gamma}(s)\omega_0}{\pi}(p-q)t\right) \right. \\ &\quad \left. + Im(\rho_{12}^*\nu_{12}) \cos\left(\chi_c^2\frac{\tilde{\Gamma}(s)\omega_0}{\pi}(p-q)t\right) \right\} \end{aligned} \quad (4.59)$$

$$\overline{W}(t) = \left\{ (p-q)^2 + e^{-2\chi_l^2\tilde{\Gamma}_l} \left[ |\rho_{12}|^2 + |\nu_{12}|^2 - 2Re\left(\rho_{12}^*\nu_{12}e^{i\chi_c^2\overline{S}(t)(p-q)}\right) \right] \right\}^{1/2} \quad (4.60)$$

and

$$\overline{\sigma}(t, \rho(t), \nu(t)) = \frac{\overline{Z}(t)}{\overline{W}(t)}. \quad (4.61)$$

Define

$$g := e^{-2\chi_l^2\frac{\tilde{\Gamma}(s-1)}{\pi}} \quad (4.62)$$

$$c := Re(\rho_{12}^*(0)\nu_{12}(0)) \quad (4.63)$$

$$d := Im(\rho_{12}^*(0)\nu_{12}(0)) \quad (4.64)$$

$$\theta := \chi_c^2\frac{\tilde{\Gamma}(s)\omega_0}{\pi}(p-q). \quad (4.65)$$

We then write

$$\overline{\sigma}(t, \rho, \nu) = \frac{\theta g(c \sin \theta t + d \cos \theta t)}{\overline{D}(t, \rho, \nu)}. \quad (4.66)$$

Using (see for example [7] p. 83) and  $\text{sgn}$  being the Signum function

$$a \cos \kappa + b \sin \kappa = \text{sgn}(a) \sqrt{a^2 + b^2} \cos \left( \kappa + \arctan \left( -\frac{b}{a} \right) \right) \quad (4.67)$$

and defining

$$\delta := \arctan \left( \frac{d}{c} \right), \quad c \neq 0, \quad (4.68)$$

we have

$$\bar{\sigma}(t, \rho, \nu) = \frac{\theta \cdot g \cdot \text{sgn}(c) \sqrt{c^2 + d^2} \cos(\theta t - \delta)}{\bar{D}(t, \rho, \nu)} \quad (4.69)$$

with the trace distance for large  $t$  being

$$\bar{D}(t, \rho, \nu) = \left\{ (p - q)^2 + g \cdot \left( |\rho_{12}|^2 + |\nu_{12}|^2 - 2 \text{sgn}(c) \sqrt{c^2 + d^2} \cos(\theta t + \delta) \right) \right\}^{1/2}. \quad (4.70)$$

We then have for the asymptotic non-Markovianity  $\bar{N}(\Phi)$

$$\bar{N}(\Phi) = \max_{\rho(0), \nu(0)} \int_{\bar{\sigma} > 0} \bar{\sigma}(t, \rho(0), \nu(0)) dt. \quad (4.71)$$

Using the asymptotic notations (4.55)-(4.58),  $|e^{1/t} - 1| \geq 2/t$  for  $t$  sufficiently large and  $s > 1$  we find

$$e^{-\Gamma_l(t)} = e^{\bar{\Gamma}_l} + O(t^{1-s}) \quad (4.72)$$

$$\sin(\tau S(t)) = \sin(\tau \bar{S}(t)) + O(t^{1-s}) \quad (4.73)$$

$$\cos(\tau S(t)) = \cos(\tau \bar{S}(t)) + O(t^{1-s}), \quad (4.74)$$

where  $\tau = \chi_c^2(p - q)$ . Using this we can write (see page 63)

$$|v(t)|^2 = e^{-2\chi_l^2 \Gamma_l(t)} \left( |\rho_{12}|^2 + |\nu_{12}|^2 - 2c \cos(\tau S(t)) + 2d \sin(\tau S(t)) \right) \quad (4.75)$$

$$= e^{-2\chi_l^2 \bar{\Gamma}_l} \left( |\rho_{12}|^2 + |\nu_{12}|^2 - 2c \cos(\tau \bar{S}(t)) + 2d \sin(\tau \bar{S}(t)) \right) + O(t^{1-s}) \quad (4.76)$$

$$= g \left( |\rho_{12}|^2 + |\nu_{12}|^2 - 2 \text{sgn}(c) \sqrt{c^2 + d^2} \cos(\theta t + \delta) \right) + O(t^{1-s}) \quad (4.77)$$

Thus we can write, see (4.70)

$$D(t, \rho, \nu) = \sqrt{(p - q)^2 + |v(t)|^2} = \bar{D}(t, \rho, \nu) + O(t^{1-s}). \quad (4.78)$$

For  $Z(t)$  (see (4.30)) we use the same approach and with  $\gamma(t) = O(t^{-s})$  we have

$$\gamma(t)|v(t)|^2 = O(t^{-s}). \quad (4.79)$$

We can thus write using (4.69)

$$\sigma(t, \rho, \nu) = \bar{\sigma}(t, \rho, \nu) + O(t^{1-s}) = \frac{\theta \cdot g \cdot \text{sgn}(c) \sqrt{c^2 + d^2} \cos(\theta t - \delta)}{\bar{D}(t, \rho, \nu)} + O(t^{1-s}). \quad (4.80)$$

We will need to consider different cases depending on the off-diagonals  $\rho_{12}(0)$  and  $\nu_{12}(0)$  having a real and/or complex component. We will also assume  $\chi_c \neq 0$  from here on as otherwise the  $N_{\text{tot}}$  particle system is not coupled to the collective reservoir. We have four cases to consider for  $c = \text{Re}(\rho_{12}^*(0)\nu_{12}(0))$  and  $d = \text{Im}(\rho_{12}^*(0)\nu_{12}(0))$ :

1.  $c \neq 0$  and  $d = 0$
2.  $c = 0$  and  $d \neq 0$
3.  $c \neq 0$  and  $d \neq 0$
4.  $c = 0$  and  $d = 0$

### 4.3 Main Result

We will show that for the case when we have an averaged effect from all spins on a single spin, 1. – 3., that for all initial spins, all coupling constants  $\chi_l$ , all coupling constants  $\chi_c \neq 0$  and for all  $s > 1$  we have a diverging non-Markovianity  $N(\Phi)$ . For  $c = d = 0$  we can identify the time evolution of the spins with the system of a single spin coupled to a bosonic field, same as section 2.3. To show our result we invoke Theorem 4.3.2 below. The assumptions (4.86) - (4.88) from the main theorem 4.3.2 are verified by the figures 4.2, 4.3 and 4.4 for the three cases. We can then directly use theorem 4.3.2 to conclude  $N(\Phi) = \infty$ .

**Remark 4.3.1.** Recall that

$$N(\Phi) = \max_{\rho(0), \nu(0)} \int_{\sigma > 0} \sigma(t, \rho(0), \nu(0)) dt \quad (4.81)$$

is a maximization problem for the initial conditions  $\rho(0), \nu(0)$ . We denote the optimal state pair that maximizes  $N(\Phi)$  by  $\rho^{\text{max}}(0), \nu^{\text{max}}(0)$ . The optimal state pair must satisfy

the conditions (D.2) - (D.4). But if we find specific initial conditions  $\rho(0), \nu(0)$  satisfying

$$\int_{\sigma>0} \sigma(t, \rho(0), \nu(0)) dt = +\infty \quad (4.82)$$

but not necessarily (D.2) - (D.4) we can conclude

$$N(\Phi) \geq \int_{\sigma>0} \sigma(t, \rho(0), \nu(0)) dt = +\infty \quad (4.83)$$

and thus have an infinite non-Markovianity. This argument of course also holds for

$$\overline{N}(\Phi) = \max_{\rho(0), \nu(0)} \int_{\overline{\sigma}>0} \overline{\sigma}(t, \rho, \nu) dt. \quad (4.84)$$

With the following main theorem we can conclude a diverging non-Markovianity if the systems trace distance and rate of change fulfill certain assumptions.

**Theorem 4.3.2.** *Let  $\bar{a}_n, \bar{b}_n$  be consecutive zeros of  $\overline{\sigma}(t, \rho, \nu)$  s.t.*

$$\overline{\sigma}(t, \rho, \nu) > 0 \quad \text{for } t \in (\bar{a}_n, \bar{b}_n). \quad (4.85)$$

*Assume there is an  $n_0$  such that for all  $n > n_0$  there exist  $\xi_n > 0$  s.t.*

$$\sigma(t, \rho, \nu) > \frac{\overline{\sigma}(t, \rho, \nu)}{2} \quad \text{for } t \in (\bar{a}_n + \xi_n, \bar{b}_n - \xi_n) \quad (4.86)$$

*and*

$$\lim_{n \rightarrow \infty} \xi_n = 0. \quad (4.87)$$

*Suppose also that there is a  $\zeta > 0$  s.t. for some initial quantum pair  $\rho(0), \nu(0)$*

$$\overline{\Delta}_n = \overline{D}(\bar{b}_n, \rho, \nu) - \overline{D}(\bar{a}_n, \rho, \nu) \geq \zeta \quad , \quad n \geq n_0. \quad (4.88)$$

*Then*

$$N(\Phi) = \infty. \quad (4.89)$$

*Proof.* With  $t_0 = O(n_0)$  we have

$$\begin{aligned}
\int_{\sigma > 0} \sigma(t, \rho(0), \nu(0)) dt &\geq \int_{\cup_{n \geq n_0} (\bar{a}_n + \xi_n, \bar{b}_n - \xi_n)} \sigma(t, \rho(0), \nu(0)) dt \\
&\geq \frac{1}{2} \int_{\cup_{n \geq n_0} (\bar{a}_n + \xi_n, \bar{b}_n - \xi_n)} \bar{\sigma}(t, \rho(0), \nu(0)) dt \\
&= \frac{1}{2} \sum_{n \geq n_0} \left( \bar{D}(\bar{b}_n - \xi_n, \rho(0), \nu(0)) - \bar{D}(\bar{a}_n + \xi_n, \rho(0), \nu(0)) \right) \quad (4.90) \\
&= \frac{1}{2} \sum_{n \geq n_0} \left( \bar{\Delta}_n + O(\xi_n) \right) \\
&= \infty.
\end{aligned}$$

We thus conclude with remark 4.3.1

$$N(\Phi) = \infty. \quad (4.91)$$

■

Instead of checking the validity of (4.86) - (4.88) by using the graphs in the figures, one could reason analytically as follows. As  $v(t)$  goes to zero exponentially quickly according to (4.24),  $\bar{\sigma}(t, \rho(0), \nu(0))$  is very quickly becoming periodic in  $t$  and has periodically reoccurring maxima. The values of the maxima are independent of  $t$  and so is the length of the intervals between consecutive zeroes, for large  $t$ . From this it is immediate that one can find  $\xi_n$  that fulfills the assumptions (4.86) and (4.87). We will now show that there exist specific initial values  $\rho(0)$  and  $\nu(0)$  for cases 1. – 3. such that  $\bar{N}(\Phi) = \infty$ . We also plot  $\bar{\sigma}$  and  $\bar{N}(\Phi)$  for all four cases and can validate the assumptions (4.86) - (4.88) with figures 4.2, 4.3 and 4.4 for the systems when an averaged effect from all other spins is present. When there is no averaged effect,  $c = d = 0$ , we can identify the system with that of a single spin coupled to one bosonic field, same as section 2.3.

1.  $c \neq 0$  and  $d = 0$ .

According to (4.69) and (4.70) we can approximate  $\sigma(t, \rho, \nu)$  and the trace distance



for large  $t$  to behave like

$$\bar{\sigma}(t, \rho, \nu) = \frac{\theta \cdot g \cdot c \cdot \sin(\theta t)}{\bar{D}(t, \rho, \nu)} \quad (4.92)$$

$$\bar{D}(t, \rho, \nu) = \left\{ (p - q)^2 + g \cdot \left( |\rho_{12}|^2 + |\nu_{12}|^2 - 2c \cos(\theta t) \right) \right\}^{1/2}. \quad (4.93)$$

Keeping the constraints (D.2) - (D.4) from appendix D in mind choose

$$p = 0.8 \quad q = 0.2 \quad \rho_{12} = 0.4 \quad \nu_{12} = -0.4. \quad (4.94)$$

It follows that

$$\theta > 0, \quad c = -0.16. \quad (4.95)$$

Consequently the  $n$ -th root  $x_n$  of  $\bar{\sigma}$  is given by

$$x_n = \frac{n\pi}{\theta}, \quad n \in \mathbb{N}_0. \quad (4.96)$$

Calculating  $\bar{D}(t, \rho(t), \nu(t))$  for  $t = x_{2n-1}$  and  $t = x_{2n}$  with

$$x_{2n-1} = \frac{(2n-1)\pi}{\theta} \quad (4.97)$$

$$x_{2n} = \frac{2n\pi}{\theta} \quad (4.98)$$

results in

$$\bar{D}(x_{2n}, \rho, \nu) = \left\{ (p - q)^2 + g \cdot \left( |\rho_{12}|^2 + |\nu_{12}|^2 - 2c \cos(2n\pi) \right) \right\}^{1/2} \quad (4.99)$$

$$\bar{D}(x_{2n-1}, \rho, \nu) = \left\{ (p - q)^2 + g \cdot \left( |\rho_{12}|^2 + |\nu_{12}|^2 - 2c \cos((2n-1)\pi) \right) \right\}^{1/2}. \quad (4.100)$$

This gives (note that  $c = -0.16 < 0$ )

$$\bar{\sigma}(t, \rho, \nu) > 0 \Leftrightarrow t \in (x_{2n-1}, x_{2n}) \text{ for } n \in \mathbb{N} \quad (4.101)$$

and using equations (4.99) and (4.100) we have

$$\overline{D}(x_{2n}, \rho, \nu) = \sqrt{0.36 + g(0.32 + 0.32 \cos(2n\pi))} = \sqrt{0.36 + 0.64g} \quad (4.102)$$

$$\overline{D}(x_{2n-1}, \rho, \nu) = \sqrt{0.36 + (0.32 + 0.32 \cos((2n-1)\pi))} = 0.6. \quad (4.103)$$

Since  $g = e^{-2\chi_l^2 \tilde{\Gamma}(s-1)/\pi} > 0$  it follows that for all  $n \in \mathbb{N}$

$$\overline{D}(x_{2n}, \rho, \nu) > \overline{D}(x_{2n-1}, \rho, \nu) \quad \forall \chi_l \in \mathbb{R}, \forall \omega_0, \chi_c \in \mathbb{R} \setminus 0 \text{ and } \forall s > 1. \quad (4.104)$$

We then have for all  $g$

$$\overline{\Delta}_n = \overline{D}(x_{2n}, \rho, \nu) - \overline{D}(x_{2n-1}, \rho, \nu) = \sqrt{0.36 + 0.64g} - 0.6 > 0. \quad (4.105)$$

Thus for the initial quantum states  $\rho(0) = \begin{pmatrix} 0.8 & 0.4 \\ 0.4 & 0.2 \end{pmatrix}$ ,  $\nu(0) = \begin{pmatrix} 0.2 & -0.4 \\ -0.4 & 0.8 \end{pmatrix}$  we can calculate  $\overline{N}(\Phi)$  using remark 4.3.1

$$\overline{N}(\Phi) = \sum_{n \geq 1} \overline{D}(x_{2n}, \rho, \nu) - \overline{D}(x_{2n-1}, \rho, \nu) \quad (4.106)$$

$$= \sum_{n \geq 1} \sqrt{0.36 + 0.64g} - 0.6 \quad (4.107)$$

$$= +\infty. \quad (4.108)$$

In figure 4.2 we see plotted  $\overline{\sigma}(t, \rho, \nu)$  and  $\overline{D}(t, \rho, \nu)$  for the initial values (4.94). We see here that  $\overline{\sigma}(t, \rho, \nu)$  is periodic and becomes very positive quickly in all intervals  $(\bar{a}_n, \bar{b}_n)$  compared to  $O(t^{1-s})$ . We can thus choose  $\xi_n = O(n^{1-s})$  and this together with (4.105) fulfills assumptions (4.86)-(4.88).

2.  $c = 0$  and  $d \neq 0$ .

According to (4.61) we can approximate  $\sigma(t, \rho, \nu)$  and the trace distance for large  $t$  by

$$\overline{\sigma}(t, \rho, \nu) = \frac{\theta \cdot g \cdot d \cdot \cos(\theta t)}{\overline{D}(t, \rho, \nu)} \quad (4.109)$$

$$\overline{D}(t, \rho, \nu) = \left\{ (p - q)^2 + g \cdot \left( |\rho_{12}|^2 + |\nu_{12}|^2 + 2d \sin(\theta t) \right) \right\}^{1/2}. \quad (4.110)$$

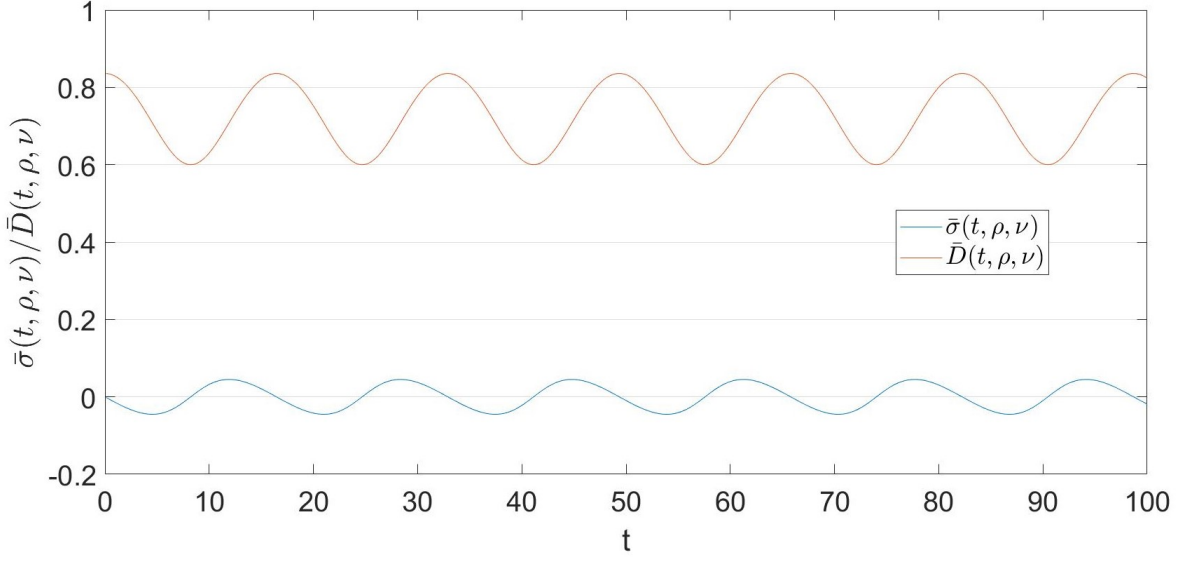


Figure 4.2: Trace distance and rate of change for  $c \neq 0$  and  $d = 0$

Graph of the asymptotic trace distance  $\bar{D}(t, \rho, \nu)$  and  $\bar{\sigma}(t, \rho, \nu)$  for  $t \in (0, 100)$  and the initial values  $p = 0.8, q = 0.2, \rho_{12} = 0.4, \nu_{12} = -0.4$  and  $s = 3, \omega_0 = \chi_c = \chi_l = 1$ .

Choosing

$$p = 0.8 \quad q = 0.2 \quad \rho_{12} = i0.4 \quad \nu_{12} = -0.4, \quad (4.111)$$

results in

$$\theta > 0, \quad d = \text{Im}(\rho_{12}^* \nu_{12}) = +0.16. \quad (4.112)$$

Consequently the  $n$ -th root  $x_n$  of  $\bar{\sigma}$  is given by

$$x_n = \frac{(2n+1)\pi}{2\theta}, \quad n \in \mathbb{N}_0 \quad (4.113)$$

and we have

$$\bar{\sigma}(t, \rho, \nu) > 0 \Leftrightarrow t \in (x_{2n+1}, x_{2n+2}), \quad n \in \mathbb{N}. \quad (4.114)$$

Calculating  $\bar{D}(t, \rho(t), \nu(t))$  for  $t = x_{2n+1}$  and  $t = x_{2n+2}$  with

$$x_{2n+1} = \frac{(4n+3)\pi}{2\theta} \quad (4.115)$$

$$x_{2n+2} = \frac{(4n+5)\pi}{2\theta} \quad (4.116)$$

results in

$$\overline{D}(x_{2n+1}, \rho, \nu) = \sqrt{0.36 + g(0.32 + 0.32 \sin(\frac{3}{2}\pi))} = 0.6 \quad (4.117)$$

$$\overline{D}(x_{2n+2}, \rho, \nu) = \sqrt{0.36 + g(0.32 + 0.32 \sin(\frac{5}{2}\pi))} = \sqrt{0.36 + 0.64g}. \quad (4.118)$$

Again we have for all  $n \in \mathbb{N}$

$$\overline{D}(x_{2n+2}, \rho, \nu) > \overline{D}(x_{2n+1}, \rho, \nu) \quad \forall \chi_l \in \mathbb{R}, \forall \omega_0, \chi_c \in \mathbb{R} \setminus 0 \text{ and } \forall s > 1. \quad (4.119)$$

It follows that for all  $g$

$$\overline{\Delta}_n = \sqrt{0.36 + 0.64g} - 0.6 > 0. \quad (4.120)$$

For the asymptotic behavior for  $N(\Phi)$  we calculate

$$\begin{aligned} \overline{N}(\Phi) &= \sum_{n \geq 1} \overline{D}(x_{2n+2}, \rho, \nu) - \overline{D}(x_{2n+1}, \rho, \nu) \\ &= \sum_{n \geq 1} \sqrt{0.36 + 0.64g} - 0.6 \\ &= +\infty. \end{aligned} \quad (4.121)$$

In figure 4.3 we see plotted  $\overline{\sigma}(t, \rho, \nu)$  and  $\overline{D}(t, \rho, \nu)$  for the initial values (4.111). As in the first case, we see that  $\overline{\sigma}(t, \rho, \nu)$  is periodic and becomes very positive quickly in all intervals  $(\bar{a}_n, \bar{b}_n)$  compared to  $O(t^{1-s})$ . We can thus choose again  $\xi_n = O(n^{1-s})$  and this together with (4.120) fulfills assumptions (4.86)-(4.88).

3.  $c \neq 0$  and  $d \neq 0$

According to (4.69) and (4.70) we have

$$\overline{\sigma}(t, \rho, \nu) = \frac{\theta \cdot g \cdot \operatorname{sgn}(c) \sqrt{c^2 + d^2} \cos(\theta t - \delta)}{\overline{D}(t, \rho, \nu)} \quad (4.122)$$

and

$$\overline{D}(t, \rho, \nu) = \left\{ (p-q)^2 + g \cdot \left( |\rho_{12}|^2 + |\nu_{12}|^2 - 2 \operatorname{sgn}(c) \sqrt{c^2 + d^2} \cos(\theta t + \delta) \right) \right\}^{1/2}. \quad (4.123)$$

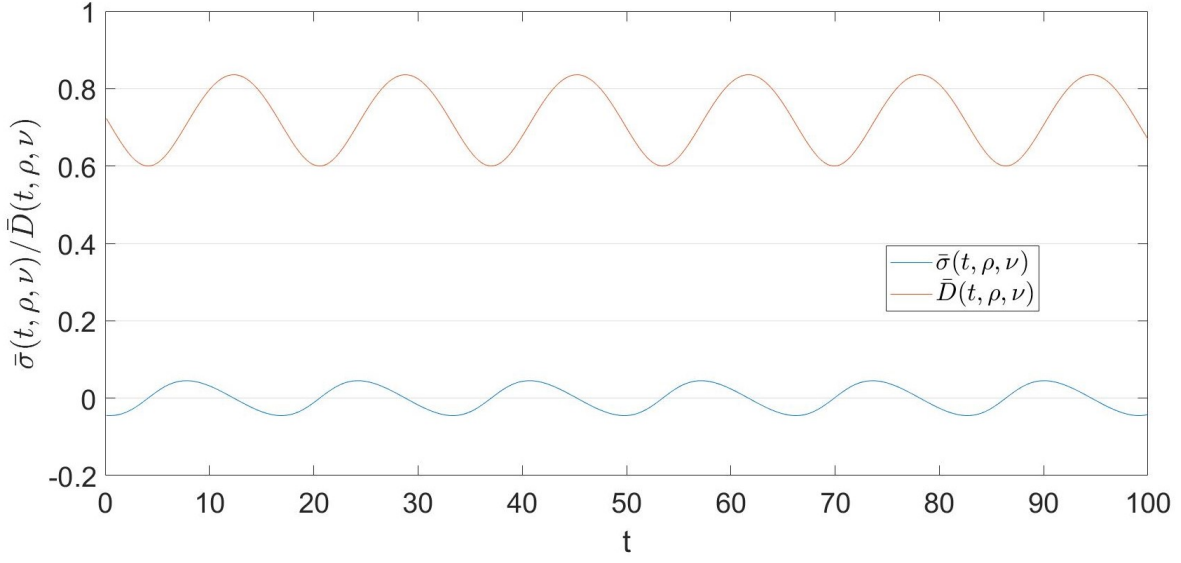


Figure 4.3: Trace distance and rate of change for  $c = 0$  and  $d \neq 0$

Graph of the asymptotic trace distance  $\bar{D}(t, \rho, \nu)$  and  $\bar{\sigma}(t, \rho, \nu)$  for  $t \in (0, 100)$  and the initial values  $p = 0.8, q = 0.2, \rho_{12} = i0.4, \nu_{12} = -0.4$  and  $s = 3, \omega_0 = \chi_c = \chi_l = 1$ .

Letting  $\rho_{12}(0) = e + if$  and  $\nu_{12}(0) = m + in$  it is

$$c = em + fn \quad (4.124)$$

$$d = en - fm. \quad (4.125)$$

Choosing

$$p = 0.8 \quad q = 0.2 \quad e = \sqrt{0.08} \quad f = 0.1 \quad m = 0.4 \quad n = 0, \quad (4.126)$$

we calculate

$$\begin{aligned} c &= \sqrt{0.08} \cdot 0.4 & d &= -0.04 & c^2 &= 0.0128 & d^2 &= 0.0016 \\ |\rho_{12}(0)|^2 &= 0.09 & |\nu_{12}(0)|^2 &= 0.16. \end{aligned} \quad (4.127)$$

With  $\theta > 0$  we calculate the roots of  $\bar{\sigma}(t, \rho, \nu)$  to be given by

$$x_n = \frac{(2n+1)\pi}{2\theta} + \frac{\delta}{\theta}. \quad (4.128)$$

With these values we have

$$\bar{\sigma}(t, \rho, \nu) > 0 \quad \text{for } t \in (x_{2n+1}, x_{2n+2}) \quad (4.129)$$

and the interval boundaries are given by

$$x_{2n+1} = \frac{(4n+3)\pi}{2\theta} + \frac{\delta}{\theta} \quad (4.130)$$

$$x_{2n+2} = \frac{(4n+5)\pi}{2\theta} + \frac{\delta}{\theta}. \quad (4.131)$$

With

$$\cos(\theta x_{2n+1} + \delta) = \cos\left(\frac{3\pi}{2} + 2\delta\right) = \sin(2\delta) \quad (4.132)$$

$$\cos(\theta x_{2n+2} + \delta) = \cos\left(\frac{5\pi}{2} + 2\delta\right) = -\sin(2\delta) \quad (4.133)$$

we have

$$\bar{D}(x_{2n+1}, \rho, \nu) = \left\{ (p-q)^2 + g\left(|\rho_{12}|^2 + |\nu_{12}|^2 - 2\text{sgn}(c)\sqrt{c^2 + d^2}\sin(2\delta)\right) \right\}^{1/2} \quad (4.134)$$

$$\bar{D}(x_{2n+2}, \rho, \nu) = \left\{ (p-q)^2 + g\left(|\rho_{12}|^2 + |\nu_{12}|^2 + 2\text{sgn}(c)\sqrt{c^2 + d^2}\sin(2\delta)\right) \right\}^{1/2}. \quad (4.135)$$

We now choose specific initial states to show that the non-Markovianity is infinite.

$$\rho(0) = \begin{pmatrix} 0.8 & \sqrt{0.08} + i0.1 \\ \sqrt{0.08} - i0.1 & 0.2 \end{pmatrix} \quad (4.136)$$

$$\nu(0) = \begin{pmatrix} 0.2 & 0.4 \\ 0.4 & 0.8 \end{pmatrix} \quad (4.137)$$

and with  $\delta = \arctan(d/c) \in (0, \pi/2)$  and  $c > 0$  we calculate according to (4.134) and (4.135)

$$\bar{D}(x_{2n+1}, \rho, \nu) = \sqrt{0.36 + g(0.25 - 0.24\sin(2\delta))} \quad (4.138)$$

$$\bar{D}(x_{2n+2}, \rho, \nu) = \sqrt{0.36 + g(0.25 + 0.24\sin(2\delta))}. \quad (4.139)$$

Recall now that  $\delta$  is fixed and  $\sin(2\delta) \in (0, 1)$ . It then follows that

$$\overline{D}(x_{2n+2}) > \overline{D}(x_{2n+1}), \quad \forall g = e^{-\chi_l^2 \frac{\Gamma(s-1)}{\pi}}. \quad (4.140)$$

As  $g$  is fixed we have that for all  $n \in \mathbb{N}$

$$\overline{\Delta}_n = \sqrt{0.36 + g(0.25 + 0.24 \sin(2\delta))} - \sqrt{0.36 + g(0.25 - 0.24 \sin(2\delta))} > 0. \quad (4.141)$$

Calculating the asymptotic non-Markovianity  $\overline{N}(\Phi)$  results in

$$\begin{aligned} \overline{N}(\Phi) &= \sum_{n \geq 1} \overline{D}(x_{2n+2}) - \overline{D}(x_{2n+1}) \\ &= \sum_{n \geq 1} \sqrt{0.36 + g(0.25 + 0.24 \sin(2\delta))} - \sqrt{0.36 + g(0.25 - 0.24 \sin(2\delta))} \\ &= +\infty. \end{aligned} \quad (4.142)$$

In figure 4.3 we see plotted  $\overline{\sigma}(t, \rho, \nu)$  and  $\overline{D}(t, \rho, \nu)$  for the initial values (4.126). Again we see that  $\overline{\sigma}(t, \rho, \nu)$  is periodic and becomes very positive quickly in all intervals  $(\bar{a}_n, \bar{b}_n)$  compared to  $O(t^{1-s})$ . We can thus choose  $\xi_n = O(n^{1-s})$  and this together with (4.141) fulfills assumptions (4.86)-(4.88).

#### 4. $c = 0$ and $d = 0$

This means that either  $\rho_{12}(0) = 0$  or  $\nu_{12}(0) = 0$ . W.l.o.g. choose  $\nu_{12}(0) = 0$ . It follows that the density matrix  $\nu$  is stationary, i.e.  $\nu(t) = \nu(0)$  for all  $t$ , see (4.14). According to (4.26) and (4.25) we have for  $\sigma$  and the trace distance  $D$  (not approximated for large  $t$ )

$$\sigma(t, \rho, \nu) = \frac{-\chi_l^2 \gamma(t) |\rho_{12}|^2 e^{-2\chi_l^2 \Gamma_l(t)}}{\sqrt{(p-q)^2 + |\rho_{12}|^2 e^{-2\chi_l^2 \Gamma_l(t)}}} \quad (4.143)$$

$$D(t, \rho, \nu) = \sqrt{(p-q)^2 + |\rho_{12}|^2 e^{-2\chi_l^2 \Gamma_l(t)}}. \quad (4.144)$$

This is the same as the situation of a single spin coupled to a bosonic field.

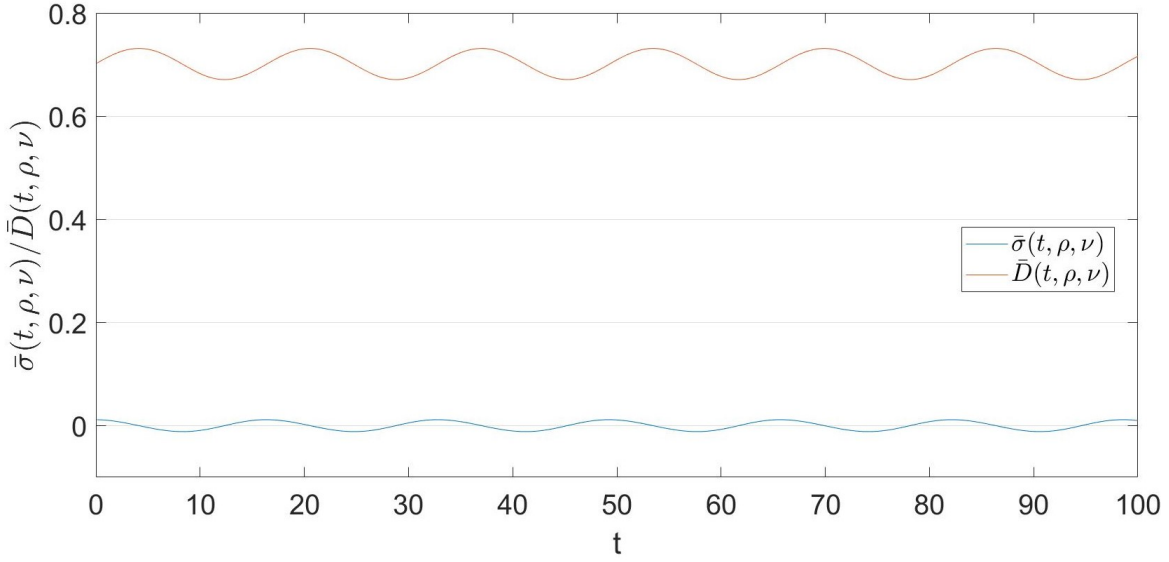


Figure 4.4: Trace distance and rate of change for  $c \neq 0$  and  $d \neq 0$

Graph of the asymptotic trace distance  $\bar{D}(t, \rho, \nu)$  and  $\bar{\sigma}(t, \rho, \nu)$  for  $t \in (0, 100)$  and the initial values  $p = 0.8, q = 0.2, \rho_{12} = \sqrt{0.08} + i0.1, \nu_{12} = 0.4$  and  $s = 3, \omega_0 = \chi_c = \chi_l = 1$ .

Comparing (4.143) and (3.61) from section 3.3 we see that we have

$$\alpha = \rho_{11} - \nu_{11} = (p - q) \quad (4.145)$$

$$|v|^2 = \chi_l^2 |\rho_{12}|^2. \quad (4.146)$$

We have shown on page 43 that if  $\sigma(t, \rho(0), \nu(0))$  is of the form (3.61) that the optimal state pair for which maximization is reached in

$$N(\Phi) = \max_{\rho(0), \nu(0)} \int_{\sigma > 0} \sigma(t, \rho(0), \nu(0)) dt \quad (4.147)$$

is given by any two initial states  $\rho(0), \nu(0)$  that satisfy

$$\alpha = p - q = 0 \text{ and } |v|^2 = \chi_l^2 |\rho_{12}|^2 = 1. \quad (4.148)$$

In particular, we have  $p = q$  and the analysis is the same as for a single spin coupled to the Bose field, hence we have

$$\sigma(t, \rho(t), \nu(t)) = -\chi_l^2 |\rho_{12}(0)| \gamma(t) e^{-\chi_l^2 \Gamma(t)}. \quad (4.149)$$



Here we have the additional coupling constant  $\chi_l$  to the local reservoir. Section 3.3 then is the special case for  $\chi_l = 1$ . Note that here as in section 3.3, in contrast to the other cases, we have a dependency of the parameter  $s$ , we denote this by using the superscript  $s$  in the functions  $\gamma_l^s(t)$  and  $\Gamma_l^s(t)$ .

We conclude this section by calculating a lower bound  $N_{low}(\Phi)$  with spectral density of form  $J(\omega) = \frac{\omega^s}{\omega_0^{s-1}} e^{-\frac{\omega}{\omega_0}}$  for the specific value  $s = 3$  and showing in particular that it is strictly positive. Choose initial values

$$p = 0.5, \quad q = 0.4 \quad \rho_{12} = 0.5 \quad \nu_{12} = 0. \quad (4.150)$$

Note that these values do not satisfy the constraints (D.2)-(D.4) for an optimal state pair and thus we only have a lower bound for the non-Markovianity  $N(\Phi)$ . We now have the initial quantum states  $\rho(0) = \begin{pmatrix} 0.5 & 0.5 \\ 0.5 & 0.5 \end{pmatrix}, \nu(0) = \begin{pmatrix} 0.4 & 0 \\ 0 & 0.6 \end{pmatrix}$ .

Using the information from section 3.3 with a spectral density of form  $J(\omega) = \frac{\omega^s}{\omega_0^{s-1}} e^{-\frac{\omega}{\omega_0}}$ , pages 53 and following, we can calculate a lower bound  $N_{low}(\Phi)$

$$\begin{aligned} N_{low}(\Phi) &= \int_{\sigma > 0} \sigma(t, \rho, \nu) dt \\ &= \sum_n D(b_n, \rho, \nu) - D(a_n, \rho, \nu), \end{aligned} \quad (4.151)$$

where again  $(a_n, b_n)$  are the intervals such that  $\sigma > 0$ . For example for  $2 < s \leq 4$  (see page 54) we have one interval such that  $\sigma > 0$  and we can calculate:

$$a_1 = \frac{\tan(\frac{\pi}{s})}{\omega_0}, \quad b_1 = \infty \quad (4.152)$$

$$\Gamma_l(a_1) = \frac{\tilde{\Gamma}(s-1)}{\pi} (1 + \cos^s(\frac{\pi}{s})) \quad (4.153)$$

$$\Gamma_l(b_1) = \frac{\tilde{\Gamma}(s-1)}{\pi} \quad (4.154)$$

and for  $s = 3$  we have

$$\gamma_l^3(t) = \frac{2\omega_0}{\pi(t^2\omega_0^2 + 1)^{\frac{3}{2}}} \sin(3 \arctan(t\omega_0)) \quad (4.155)$$

$$\Gamma_l^3(t) = \frac{2}{\pi} \left( 1 - \frac{\cos(2 \arctan(t\omega_0))}{(t^2\omega_0^2 + 1)} \right). \quad (4.156)$$

It follows

$$\begin{aligned} N_{low}(\Phi) &= D(b_1, \rho, \nu) - D(a_1, \rho, \nu) \\ &= \sqrt{0.01 + 0.25e^{-\chi_l^2 \frac{2}{\pi}}} - \sqrt{0.01 + 0.25e^{-\chi_l^2 \frac{2.25}{\pi}}} \\ &> 0, \quad \forall \chi_l \neq 0. \end{aligned} \quad (4.157)$$

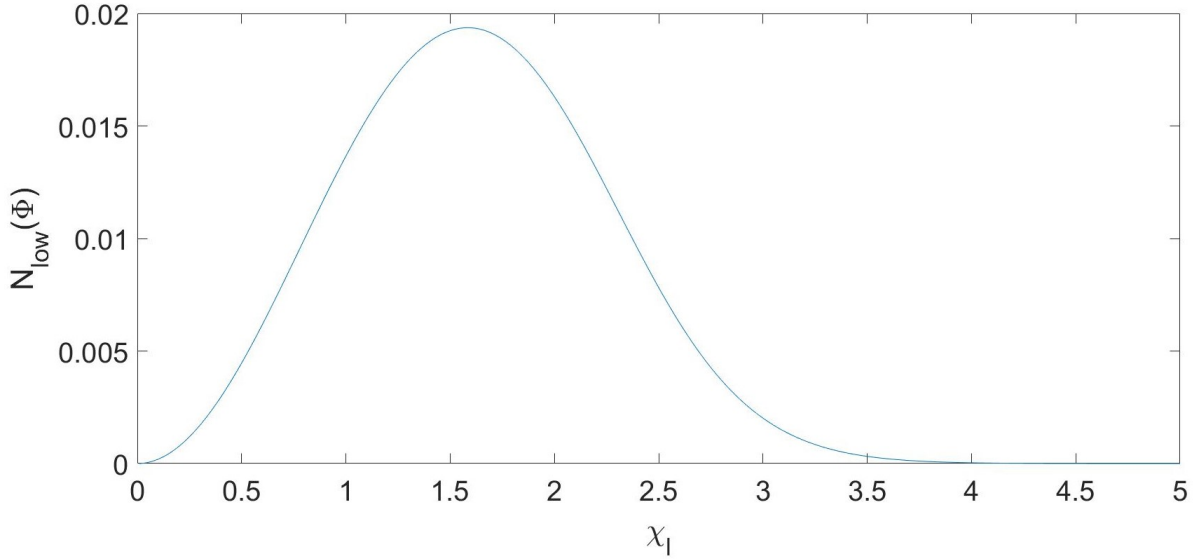


Figure 4.5:  $N_{low}(\Phi)$  for  $c = d = 0$

$N_{low}(\Phi)$  for  $0 < \chi_l \leq 5$  for  $p = 0.5$ ,  $q = 0.4$ ,  $\rho_{12} = 0.5$  and  $\nu_{12} = 0$

It is interesting to note that for very small and very large coupling constant, the non-Markovianity is suppressed and it attains its maximum for an intermediate value for the coupling constant, see Figure 4.5. Note that this is a lower bound for the non-Markovianity and not an optimal state pair, which would be  $p = q$ . Nevertheless, it shows that the process is non-Markovian.

We can already see in (4.143) that  $\sigma$  does not depend on the coupling constant  $\chi_c$  to the common reservoir. Also by comparison with section 3.3 we see that with the

identifications (4.145) and (4.146) we can identify the case  $c = d = 0$  with a single spin coupled to a bosonic field. Thus only the local bosonic field has an effect on the time evolution of the spins and there is no averaged effects through the common reservoir on the spins.

## Outlook

An interesting extension of this work would be to transfer the results obtained in sections 2.3 and 3.3 to other dynamics, i.e.

- Dimer model with local and collective reservoirs (using for example the explicit density matrix form from [23])
- Perturbation theory for a spin weakly or strongly coupled to a bosonic field

and calculate the non-Markovianity  $N$  for these systems.

We have discussed solely the non-Markovianity measure based on the trace distance for the dynamics considered. As not all measures for non-Markovianity are equivalent (see [17]) it would be interesting to compare the results obtained to other measures such as divisibility measure (by Rivas, Huelga and Plenio [27]), coherent information measure (by Luo, Fu and Song [21]) and channel capacity measures (by Bylicka, Chruściński and Maniscalco [8]).

# Bibliography

- [1] C. Addis, B. Bylicka, D. Chruściński, S. Maniscalco *Comparative study of non-Markovianity measures in exactly solvable one and two qubit models* Physical Review A, **90**, 052103 (2014)
- [2] H.-P. Breuer *Foundations and measures of quantum non-Markovianity* 2012 J. Phys. B: At. Mol. Opt. Phys. **45** 154001
- [3] H.-P. Breuer *Genuine quantum trajectories for non-Markovian processes* 2004 Phys. Rev. A **70**, 012106
- [4] H.-P. Breuer, E.-M. Laine, J. Piilo, B. Vacchini *Non-Markovian dynamics in open quantum systems* 2016 Rev. Mod. Phys. **88**, 021002
- [5] H.P. Breuer, E.M. Laine, J. Piilo *Measure for the degree of Non-Markovian Behavior of Quantum Processes in Open Systems* Phys. Rev. Lett **103**, 210401 (2009)
- [6] H. -P. Breuer and F. Petruccione *The Theory of Open Quantum Systems* Oxford University Press, 2002
- [7] I.N. Bronstein et. al. *Taschenbuch der Mathematik* Harri Deutsch Verlag, 2005
- [8] B. Bylicka, D. Chruściński, S. Maniscalco *Non-Markovianity and reservoir memory of quantum channels: a quantum information theory perspective* Scientific Reports volume 4, Article number: 5720, 2014
- [9] A. G. Dijkstra, Y. Tanimura *Non-Markovianity: initial correlations and nonlinear optical measurements* Phil. Trans. R. Soc. A **370**, 3658-3671.
- [10] C. Gardiner, P. Zoller *Quantum noise* Springer Verlag, 2010
- [11] V. Gorini, A. Kossakowski, E. C. G. Sudarshan *Completely positive dynamical semigroups of  $N$ - level systems* 1976 J. Math. Phys., 821
- [12] I.S. Gradshteyn, I.M. Ryzhik *Table of integrals, series and products* Academic Press, 2007
- [13] G. Guarnieri, A. Smirne, B. Vacchini *Quantum regression and non-Markovianity of quantum dynamics* Phys. Rev. A **90**, 022110 (2014)

- [14] P. Haikka, T. Johnson, S. Maniscalco *Non-Markovianity of local dephasing channels and time-invariant discord* arXiv:1203.6469, 2012
- [15] B.C. Hall *Lie Groups, Lie Algebras, and Representations: An Elementary Introduction* Springer Verlag, 2003
- [16] M. J. W. Hall, J.D. Cresser, L.Li, E. Anderson *Canonical form of master equations and characterization of non-Markovianity* arXiv:1009.0845v4 (2014)
- [17] M. Jiang, S. Luo *Comparing quantum Markovianities: Distinguishability versus correlations* Phys. Rev. A **88**, 034101 (2013)
- [18] K. Kraus *States, Effects, and Operations: Fundamental Notions of Quantum Theory* Springer Verlag (1983)
- [19] G. Lindblad *On the Generators of Quantum Dynamical Semigroups* Comm. Math. Phys. **48**, 119 (1976)
- [20] X.-M. Lu, X. Wang, C.P. Sun *Optimal measurements to access classical correlations of two-qubit states* arXiv:1009.1476 (2011)
- [21] S. Luo, S. Fu, H. Song *Quantifying non-Markovianity via correlations* Phys. Rev. A **86**, 044101 (2012)
- [22] M. Merkli *The Ideal Quantum Gas* Spinger Lecture Notes in Mathematics **1880**, 183-233, 2006
- [23] M. Merkli et. al. *Dynamics of a Chlorophyll Dimer in Collective and Local Thermal Environments* arXiv:1512.08810, 2015
- [24] M. Merkli, G.P. Berman *Mean field evolution of open quantum systems An exactly solvable model* Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci. **468**, no. 2147, 3398-3412 (2012)
- [25] M. Mohseni, A. Shabani, S. Lloyd, Y. Omar, H. Rabitz *Geometrical effects on energy transfer in disordered open quantum systems* The Journal of Chemical Physics **138**, 204309 (2013)
- [26] M. Nielsen, I. Chuang *Quantum Computation and Quantum Information* Cambridge University Press, 2010
- [27] A. Rivas, S. F. Huelga, M. B. Plenio *Entanglement and Non-Markovianity of Quantum Evolutions* Phys. Rev. Lett. **105**, 050403 (2010)
- [28] S. Wißmann, A. Karlsson, E.-M. Laine, J. Piilo, H.-P. Breuer, *Optimal state pairs for non-Markovian quantum dynamics* 2012 Phys. Rev. A **86**, 062108

- [29] RC. Zamar, O. Mensio *Nuclear magnetic resonance proton dipolar order relaxation in thermotropic liquid crystals: a quantum theoretical approach* J Chem Phys. 2004 Dec 15;121(23):11927-41

# Appendix A

## Proposition

Let  $X$  and  $Y$  be operators on some Hilbert Space  $\mathcal{H}$ . We then have the following identities from [\[15\]](#) (Proposition 2.24. and Definition 2.22)

$$ad_X Y = [X, Y] \tag{A.1}$$

$$Ad_X Y = XYX^{-1}. \tag{A.2}$$

Proposition 2.25. states

$$e^{ad_X} Y = Ad_{e^X} Y = e^X Y e^{-X}. \tag{A.3}$$

It is

$$e^{ad_X} Y = \left( \sum_{n \geq 0} \frac{(ad_X)^n}{n!} \right) Y \tag{A.4}$$

$$= \mathbb{1}Y + ad_X Y + \frac{1}{2!}(ad_X)^2 Y + \frac{1}{3!}(ad_X)^3 Y + \dots \tag{A.5}$$

$$= Y + [X, Y] + \frac{1}{2!}[X, [X, Y]] + \frac{1}{3!}[X, [X, [X, Y]]] + \dots. \tag{A.6}$$

For  $[X, [X, Y]] = [Y, [Y, X]] = 0$  it follows from Proposition 2.25. and [\(A.6\)](#) that

$$e^X Y e^{-X} = Y + [X, Y]. \tag{A.7}$$

# Appendix B

## The Fourier Transform of the correlation function

We now introduce the "spectral density of noise"

$$J(\omega) := \sqrt{2\pi} \tanh\left(\frac{\beta\omega}{2}\right) \widehat{C}(\omega), \quad (\text{B.1})$$

where  $\widehat{C}(\omega)$  is the Fourier transform of the symmetrized correlation function

$$C(t) = \frac{1}{2} (\langle \phi_t(g) \phi(g) \rangle_\beta + \langle \phi(g) \phi_t(g) \rangle_\beta). \quad (\text{B.2})$$

We will show  $J(\omega)$  is equivalent to

$$J(\omega) = \frac{\pi}{2} \omega^2 \int_{S^2} |g(k)|^2 d\Sigma, \quad (\text{B.3})$$

where  $(\omega, \Sigma)$  are spherical coordinates on  $\mathbb{R}^3$ ,  $g(k) = g(|k|, \Sigma)$ ,  $d\Sigma$  the uniform measure over the sphere  $S_2$ . It is

$$\begin{aligned} \phi_t(g) &= e^{itH_R} \phi(g) e^{-itH_R} = \phi(e^{it\omega(k)} g) \\ &= \frac{1}{\sqrt{2}} \int_{\mathbb{R}^3} d^3k e^{it\omega(k)} g(k) a^*(k) + e^{-it\omega(k)} g^*(k) a(k) \end{aligned} \quad (\text{B.4})$$



Thus we have, as the operators  $a^*(k)a(\tilde{k})$  and  $a(k)a^*(\tilde{k})$  don't contribute

$$\begin{aligned}\langle e^{itH_R}\phi(g)e^{-itH_R}\phi(g)\rangle_\beta &= \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} d^3k d^3\tilde{k} \langle (e^{it\omega(k)}g(k)a^*(k) + \\ &\quad e^{-it\omega(k)}g^*(k)a(k))(g(\tilde{k})a^*(\tilde{k}) + g^*(\tilde{k})a(\tilde{k}))\rangle \\ &= \frac{1}{2} \int_{\mathbb{R}^3} d^3k |g(k)|^2 \left( e^{it\omega(k)}N(\omega(k)) + e^{-it\omega(k)}(N(\omega(k)) + 1) \right).\end{aligned}\tag{B.5}$$

Similarly we have, noting that  $\phi_t^*(g) = \phi_{-t}(g)$

$$\begin{aligned}\langle e^{-itH_R}\phi(g)e^{itH_R}\phi(g)\rangle_\beta &= \frac{1}{2} \int_{\mathbb{R}^3} d^3k |g(k)|^2 \left( e^{-it\omega(k)}N(\omega(k)) \right. \\ &\quad \left. + e^{it\omega(k)}(N(\omega(k)) + 1) \right),\end{aligned}\tag{B.6}$$

where  $N(k)$  is the average mode at temperature  $\beta$ . Hence it is

$$C(t) = \frac{1}{2} \int_{\mathbb{R}^3} d^3k |g(k)|^2 \left( e^{it\omega(k)}(N(\omega(k)) + \frac{1}{2}) + e^{-it\omega(k)}(N(\omega(k)) + \frac{1}{2}) \right).\tag{B.7}$$

Using

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i(\omega - \omega')t} dt = \sqrt{2\pi} \delta(\omega - \omega')\tag{B.8}$$

the Fourier transformation of (B.7) is given by

$$\begin{aligned}\widehat{C}(\omega) &= \mathcal{F}(C(t)) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega t} C(t) dt \\ &= \frac{1}{\sqrt{2\pi}} e^{-i\omega t} \int_{\mathbb{R}^3} d^3k \int_{-\infty}^{+\infty} \frac{1}{2} |g(k)|^2 \left( e^{it\omega(k)}(N(\omega(k)) + \frac{1}{2}) + \right. \\ &\quad \left. e^{-it\omega(k)}(N(\omega(k)) + \frac{1}{2}) \right) dt \\ &= \sqrt{2\pi} \int_{\mathbb{R}^3} d^3k \frac{1}{2} |g(k)|^2 \left( \delta(\omega(k) - \omega)(N(\omega(k)) + \frac{1}{2}) + \right. \\ &\quad \left. \delta(\omega + \omega(k))(N(\omega(k)) + \frac{1}{2}) \right).\end{aligned}\tag{B.9}$$

Introducing spherical coordinates  $(\omega, \Sigma)$  on  $\mathbb{R}^3$  with  $g(k) = g(|k|, \Sigma)$  and  $d\Sigma$  being the integration over the Sphere  $S^2$  we have

$$\begin{aligned}\widehat{C}(\omega) &= \sqrt{2\pi} \int_0^\infty \int_{S^2} \frac{1}{2} \omega^2(k) |g(|k|^2, \Sigma)|^2 \left( \delta(\omega(k) - \omega) (N(\omega(k)) + \tfrac{1}{2}) + \right. \\ &\quad \left. \delta(\omega + \omega(k)) (N(\omega(k)) + \tfrac{1}{2}) \right) d\omega d\Sigma \\ &= \sqrt{2\pi} \omega^2 \int_{S^2} \frac{1}{2} |g(|k|^2, \Sigma)|^2 (N(\omega) + \tfrac{1}{2}) d\Sigma.\end{aligned}\tag{B.10}$$

For a thermal reservoir we have at temperature  $\beta$

$$N(\omega) = \frac{1}{e^{\beta\omega} - 1}.\tag{B.11}$$

Also

$$\begin{aligned}\tanh\left(\frac{\beta\omega}{2}\right) \left(\frac{1}{e^{\beta\omega} - 1} + \tfrac{1}{2}\right) &= \frac{1 - e^{-\beta\omega}}{1 + e^{-\beta\omega}} \left(\frac{1}{e^{\beta\omega} - 1} + \tfrac{1}{2}\right) \\ &= \frac{1}{2},\end{aligned}\tag{B.12}$$

and so we have

$$\begin{aligned}J(\omega) &= \sqrt{2\pi} \tanh\left(\frac{\beta\omega}{2}\right) \widehat{C}(\omega) \\ &= \sqrt{2\pi} \tanh\left(\frac{\beta\omega}{2}\right) \sqrt{2\pi} \int_{S^2} \frac{1}{2} \omega^2 |g(k)|^2 \left(\frac{1}{e^{\beta\omega} - 1} + \tfrac{1}{2}\right) d\Sigma \\ &= \frac{\pi}{2} \omega^2 \int_{S^2} |g(k)|^2 d\Sigma\end{aligned}\tag{B.13}$$

with

$$\Gamma(t) = \frac{1}{\pi} \int_0^\infty J(\omega) \frac{1 - \cos(\omega t)}{\omega^2} \coth\left(\frac{\beta\omega}{2}\right) d\omega\tag{B.14}$$

$$\gamma(t) = \frac{1}{\pi} \int_0^\infty J(\omega) \frac{\sin(\omega t)}{\omega} \coth\left(\frac{\beta\omega}{2}\right) d\omega.\tag{B.15}$$

# Appendix C

## Formulas

Using reference [12] we have the following integral formulas

$$\int_0^\infty x^{s-1} e^{-\beta x} \sin(\alpha x) dx = \frac{\tilde{\Gamma}(s)}{(\alpha^2 + \beta^2)^{\frac{s}{2}}} \sin\left(s \arctan\left(\frac{\alpha}{\beta}\right)\right) \quad (\text{C.1})$$

$$\int_0^\infty x^{s-1} e^{-\beta x} \cos(\alpha x) dx = \frac{\tilde{\Gamma}(s)}{(\alpha^2 + \beta^2)^{\frac{s}{2}}} \cos\left(s \arctan\left(\frac{\alpha}{\beta}\right)\right) \quad (\text{C.2})$$

$$\int x^{s-1} \sin(\alpha x) dx = \frac{i}{2} (i\alpha)^{-s} \gamma(s, i\alpha x) - \frac{i}{2} (-i\alpha)^{-s} \gamma(s, -i\alpha x) \quad (\text{C.3})$$

$$\int_0^\infty x^n e^{-\alpha x} dx = n! \alpha^{-n-1} \quad (\text{C.4})$$

$$\int_0^\infty x^{\mu-1} e^{-\alpha x} dx = \frac{1}{\alpha^\mu} \tilde{\Gamma}(\mu) \quad [\text{Re}\alpha, \mu > 0] \quad (\text{C.5})$$

where  $\tilde{\Gamma}(s)$  is the Euler-Gamma function defined as

$$\begin{aligned} \tilde{\Gamma}(x) &= \int_0^\infty e^{-t} t^{x-1} dt \\ \gamma(\alpha, x) &= \int_0^x e^{-t} t^{\alpha-1} dt \\ \tilde{\Gamma}(\alpha, x) &= \int_x^\infty e^{-t} t^{\alpha-1} dt \\ \tilde{\Gamma}(n+1) &= n! \end{aligned}$$

# Appendix D

## Constraints

In [28] it is shown that we can reduce the possible initial quantum states  $\rho(0)$  and  $\nu(0)$  in the maximization of  $N(\Phi)$  even further. To arrive at an optimal state pair (a pair for which the maximum in equation (1.32) is reached) the initial states  $\rho(0)$  and  $\nu(0)$  must be orthogonal and lie on the boundary  $\partial S(\mathcal{H})$  of the state space  $S(\mathcal{H})$ . By definition two density matrices are orthogonal if the subspaces spanned by the eigenvectors with non-zero eigenvalues are orthogonal. This is equivalent with the condition, see [26] <sup>1</sup>

$$D(\rho(0), \nu(0)) = \sqrt{(p - q)^2 + |\rho_{12}(0) - \nu_{12}(0)|^2} = 1. \quad (\text{D.1})$$

Note also that  $D(t, \rho(t), \nu(t)) \leq 1$  for all  $t$  and since a density matrix is a positive trace class operator (compare to equation (1.3) and following) we have three restrictions on the optimal initial states  $\rho(0)$  and  $\nu(0)$ :

$$\sqrt{p(1 - p)} \geq |\rho_{12}(0)| \quad (\text{D.2})$$

$$\sqrt{q(1 - q)} \geq |\nu_{12}(0)| \quad (\text{D.3})$$

$$1 = D(\rho(0), \nu(0)) = \sqrt{(p - q)^2 + |\rho_{12}(0) - \nu_{12}(0)|^2} \quad (\text{D.4})$$

We will show now that we can also conclude  $p \neq 1$  and  $p \neq 0$  and equivalently for  $q$ . Assume  $q = 0$ .

$$\Rightarrow \nu(0) = \nu(t) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad (\text{D.5})$$

---

<sup>1</sup>p.416 equation 9.110 states  $1 - F(\rho, \nu) \leq D(\rho, \nu) \leq \sqrt{1 - F^2(\rho, \nu)}$ , where  $F(\rho, \nu)$  is the Fidelity measure. Using Uhlman's theorem one can show that  $F(\rho, \nu) = 0 \Leftrightarrow \rho$  and  $\nu$  have support on orthogonal subspaces.

Since

$$\sqrt{q(1-q)} \geq |\nu_{12}(0)|^2 \quad (\text{D.6})$$

it follows that  $\nu_{12}(0) = 0$  and then

$$1 = D(\rho(0), \nu(0)) = \sqrt{p^2 + |\rho_{12}(0)|^2}. \quad (\text{D.7})$$

$$1 = \sqrt{p^2 + |\rho_{12}(0)|^2} \quad (\text{D.8})$$

$$\leq \sqrt{p^2 + p - p^2} \quad (\text{D.9})$$

$$= \sqrt{p} \quad (\text{D.10})$$

$$\Rightarrow p = 1 \quad \text{as} \quad p \in [0, 1] \quad (\text{D.11})$$

We then have the trivial solution

$$\nu(t) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad (\text{D.12})$$

$$\rho(t) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad (\text{D.13})$$

and  $\sigma(t, \rho(t), \nu(t)) = 0$  for all  $t$ .